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 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  FEB 27   New STN AnaVist pricing effective March 1, 2006
 NEWS  4  MAY 10   CA/CAplus enhanced with 1900-1906 U.S. patent records
 NEWS  5  MAY 11   KOREAPAT updates resume
 NEWS  6  MAY 19   Derwent World Patents Index to be reloaded and enhanced
 NEWS  7  MAY 30   IPC 8 Rolled-up Core codes added to CA/CAplus and
                   USPATFULL/USPAT2
 NEWS  8  MAY 30   The F-Term thesaurus is now available in CA/CAplus
 NEWS  9  JUN 02   The first reclassification of IPC codes now complete in
                   INPADOC
 NEWS 10  JUN 26   TULSA/TULSA2 reloaded and enhanced with new search and
                   and display fields
 NEWS 11  JUN 28   Price changes in full-text patent databases EPFULL and PCTFULL
 NEWS 12  JUl 11   CHEMSAFE reloaded and enhanced
 NEWS 13  JUl 14   FSTA enhanced with Japanese patents
 NEWS 14  JUl 19   Coverage of Research Disclosure reinstated in DWPI
 NEWS 15  AUG 09   INSPEC enhanced with 1898-1968 archive
 NEWS 16  AUG 28   ADISCTI Reloaded and Enhanced
 NEWS 17  AUG 30   CA(SM)/CAplus(SM) Austrian patent law changes
 NEWS 18  SEP 11   CA/CAplus enhanced with more pre-1907 records
 NEWS 19  SEP 21   CA/CAplus fields enhanced with simultaneous left and right
                   truncation

 NEWS EXPRESS  JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

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 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
 NEWS X25      X.25 communication option no longer available

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FILE 'HOME' ENTERED AT 06:36:45 ON 23 SEP 2006

=> fil reg
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 06:36:56 ON 23 SEP 2006

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 SEP 2006 HIGHEST RN 908228-18-2
DICTIONARY FILE UPDATES: 21 SEP 2006 HIGHEST RN 908228-18-2

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http://www.cas.org/ONLINE/UG/regprops.html

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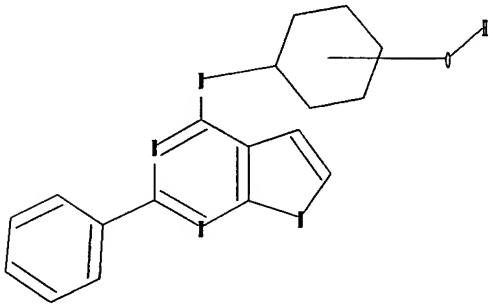

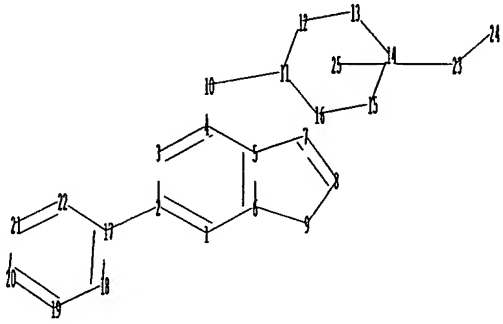

chain nodes :
10 23 24
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
2-17 4-10 10-11 23-24
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
4-10 6-9 8-9 10-11
exact bonds :
2-17 5-7 7-8 11-12 11-16 12-13 13-14 14-15 15-16 23-24
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22
isolated ring systems :
containing 1 : 11 : 17 :

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Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
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L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
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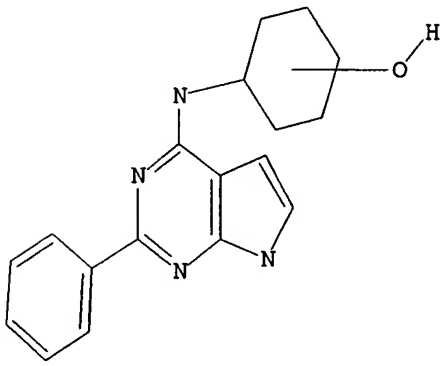


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Structure attributes must be viewed using STN Express query preparation.


=> s l1 sam
SAMPLE SEARCH INITIATED 06:37:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       27 TO ITERATE

100.0% PROCESSED       27 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          229 TO      851
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 06:37:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      547 TO ITERATE

100.0% PROCESSED      547 ITERATIONS                                37 ANSWERS
SEARCH TIME: 00.00.01

L3           37 SEA SSS FUL L1

=> s l3 and caplus/lc
      52169499 CAPLUS/LC
L4           37 L3 AND CAPLUS/LC

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   171.70     171.91
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FILE 'CAPLUS' ENTERED AT 06:37:34 ON 23 SEP 2006
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FILE COVERS 1907 - 23 Sep 2006 VOL 145 ISS 14
FILE LAST UPDATED: 22 Sep 2006 (20060922/ED)

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=> s l3
L5 13 L3

=> d l5 ibib hitstr abs 1-13

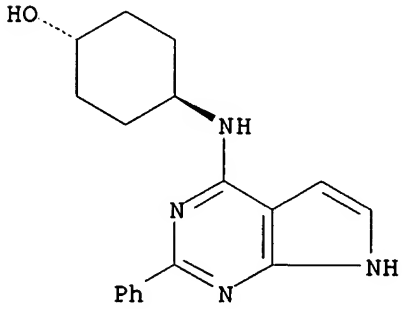
L5 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:847629 CAPLUS
DOCUMENT NUMBER: 145:278270
TITLE: Pharmaceutical compositions comprising inhibitors of neutral endopeptidase and inhibitors of the endogenous endothelin and diuretics for the treatment of cardiovascular diseases
INVENTOR(S): Witte, Klaus; Ziegler, Dieter; Straub, Matthias; Fischer, Yvan
PATENT ASSIGNEE(S): Solvay Pharmaceuticals GmbH, Germany
SOURCE: PCT Int. Appl., 39pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006087371	A1	20060824	WO 2006-EP60057	20060217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: EP 2005-101235 A 20050218

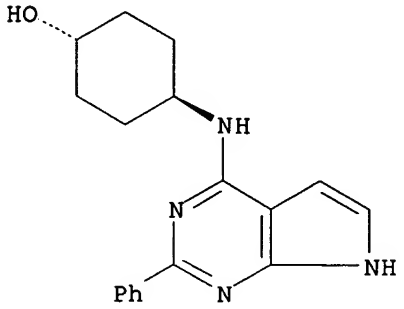
IT 251945-92-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. comprising inhibitors of neutral endopeptidase and inhibitors of the endogenous endothelin and diuretics for the treatment of cardiovascular diseases)
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 251945-92-3D, derivs.
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. comprising inhibitors of neutral endopeptidase and inhibitors of the endogenous endothelin and diuretics for the treatment of cardiovascular diseases)
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB A novel combination therapy is described for cardiovascular diseases or conditions, by administering a synergistic combination of at least one inhibitor of neutral endopeptidase, at least one inhibitor of the endogenous endothelin producing system and at least one diuretic, preferably a thiazide diuretic or an adenosine A1 antagonist. For example, capsules contained daglutril calcium, and hydrochlorothiazide, corn starch, lactose and Et acetate.
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:316276 CAPLUS
DOCUMENT NUMBER: 142:392424
TITLE: Preparation of aminopyrrolopyrimidines as adenosine A1

receptor antagonists.

INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S., 66 pp., Cont.-in-part of Appl. No. PCT/US99/12135.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6878716	B1	20050412	US 1999-454074	19991202
WO 9962518	A1	19991209	WO 1999-US12135	19990601
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2393179	AA	20010607	CA 2000-2393179	20001201
WO 2001039777	A1	20010607	WO 2000-US32702	20001201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1246623	A1	20021009	EP 2000-988011	20001201
EP 1246623	B1	20060809		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519102	T2	20030617	JP 2001-541509	20001201
AU 784878	B2	20060713	AU 2001-24270	20001201
ZA 2002004153	A	20040715	ZA 2002-4153	20020524

PRIORITY APPLN. INFO.:

US 1998-87702P	P	19980602
US 1999-123216P	P	19990308
US 1999-126527P	P	19990326
WO 1999-US12135	A2	19990601
US 1999-454074	A	19991202
US 1999-454075	A	19991202
US 1999-454254	A	19991202
WO 2000-US32702	W	20001201

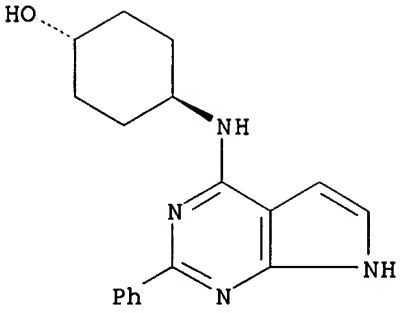
OTHER SOURCE(S): MARPAT 142:392424

IT 251945-92-3P 251946-00-6P 251946-57-3P
251946-58-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists)

RN 251945-92-3 CAPLUS

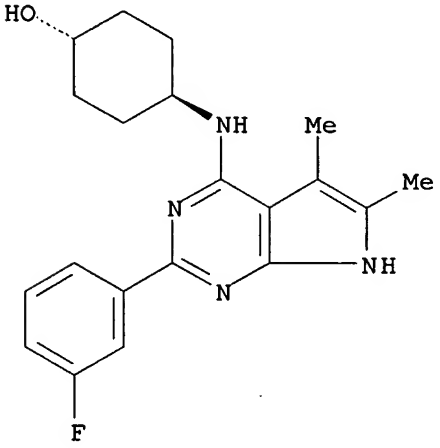
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



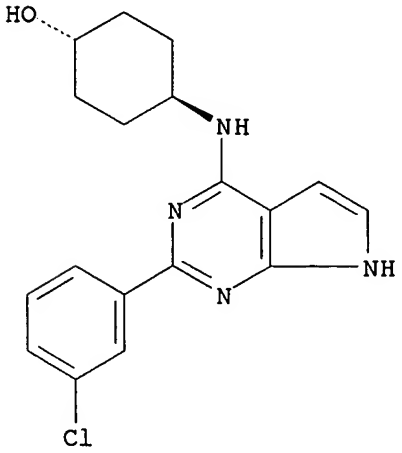
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

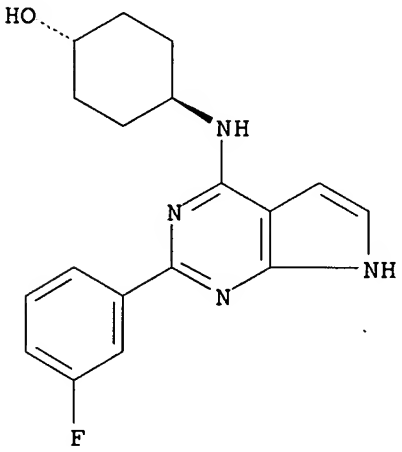
Relative stereochemistry.



RN 251946-58-4 CAPLUS

CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

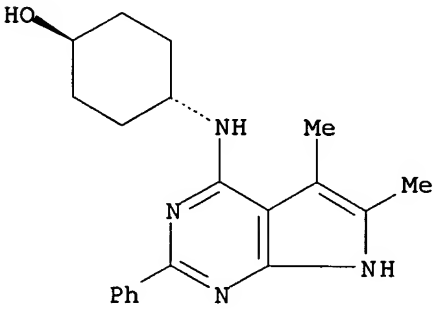
Relative stereochemistry.



IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-99-0P 251946-01-7P 251946-20-0P
343632-01-9P 343632-02-0P 343632-03-1P
343969-79-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists)

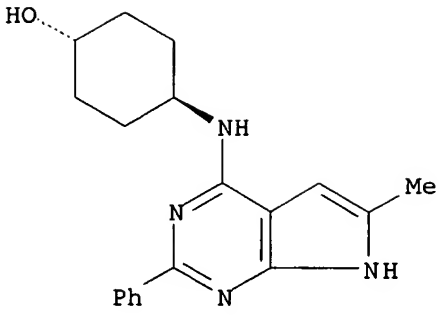
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



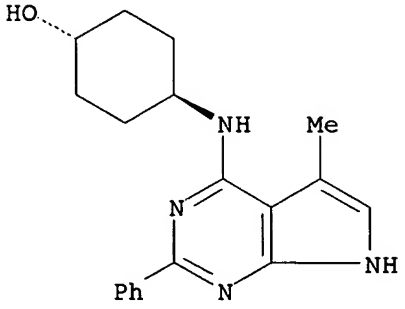
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



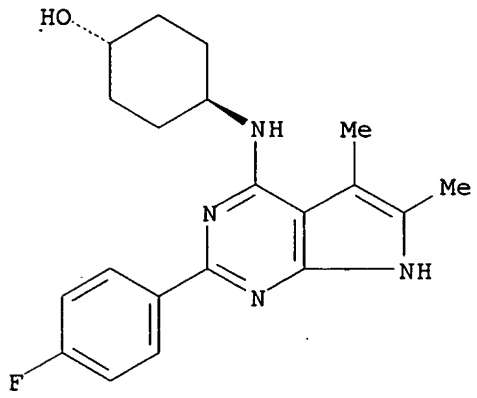
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



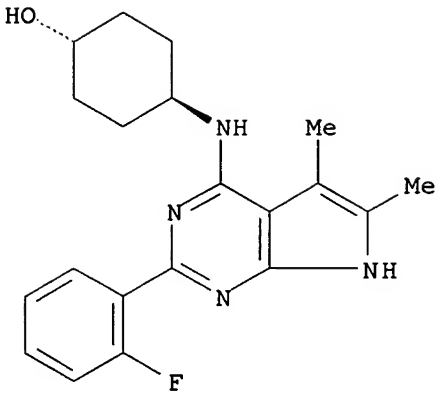
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



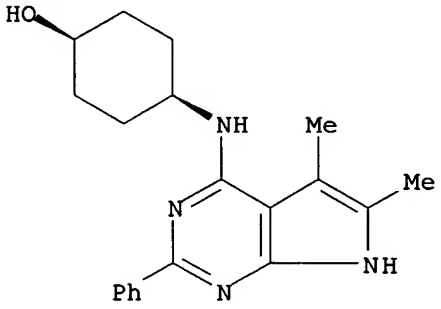
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



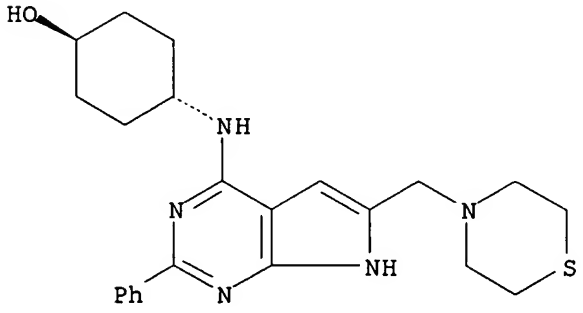
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



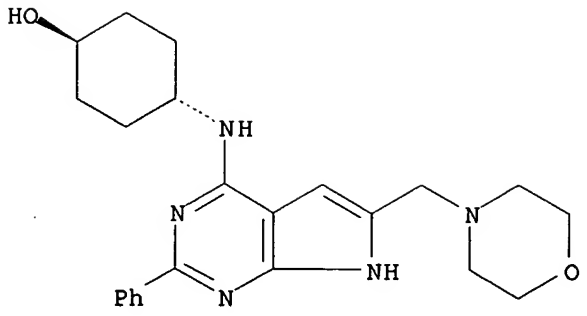
RN 343632-01-9 CAPLUS
CN Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



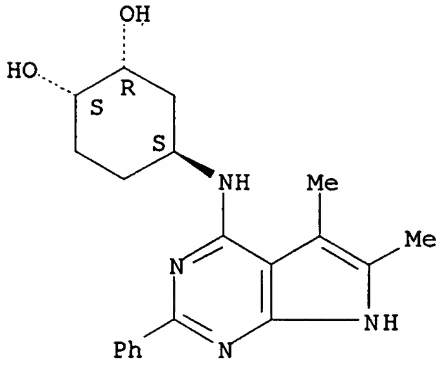
RN 343632-02-0 CAPLUS
CN Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



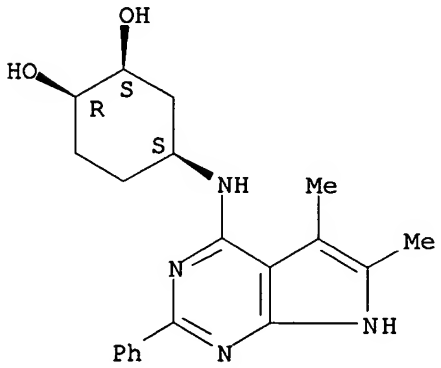
RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) (CA INDEX NAME)

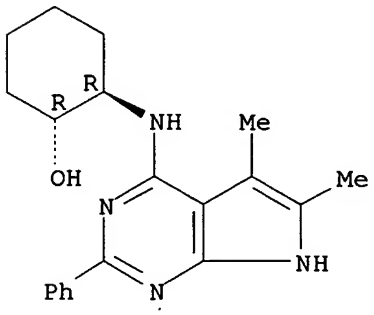
Relative stereochemistry.



IT 251946-03-9 343632-05-3 343632-07-5
849831-23-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists)
RN 251946-03-9 CAPLUS

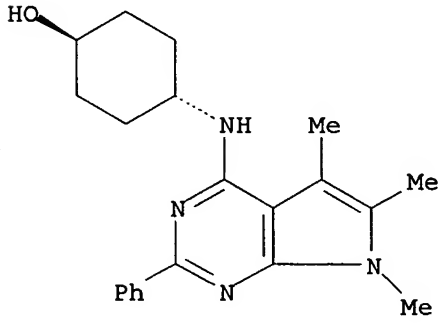
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



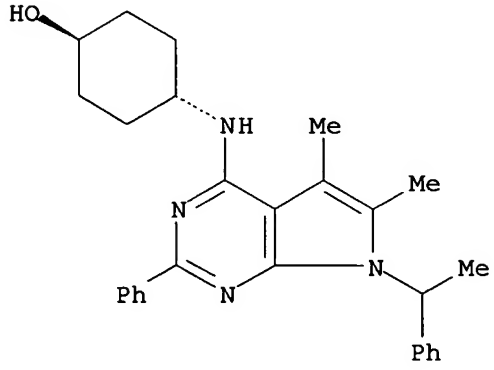
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

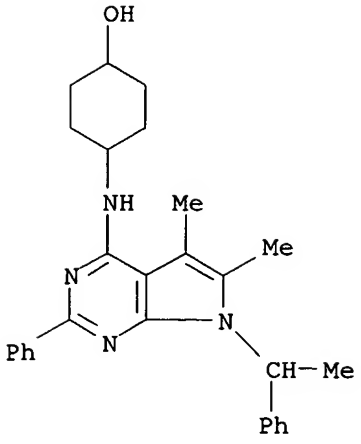


RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 849831-23-8 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]- (9CI) (CA INDEX NAME)



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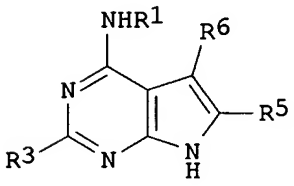


I

AB Title compds. [I; R1 = trans-4-hydroxycyclohexyl, 2-methylaminocarbonylaminocyclohexyl, acetylaminoethyl, methylaminocarbonylaminoethyl; R3 = (substituted) Ph, pyrrolyl, thienyl, furyl, thiazolyl, imidazolyl, pyrazolyl, pyrazinyl, purinyl, quinazolinyl, etc.; R5 = H, (substituted) alkyl, amino, Ph, pyrrolyl, furyl, thienyl, imidazolyl, benzoxazolyl, benzothiazolyl, triazolyl, tetrazolyl, pyrazolyl, pyridinyl, pyrazinyl, pyridazinyl, pyrimidinyl, naphthyl, quinolyl, indolyl, etc.; R6 = H, (substituted) alkyl, cycloalkyl], were prepared Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine and trans-4-hydroxycyclohexylamine were heated in Me2SO at 130° for 5 h to give 75% 4-(4-trans-hydroxycyclohexyl)amino-6-methyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine. I showed A1 receptor binding with Ki = 2.3-75000 nM.

REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

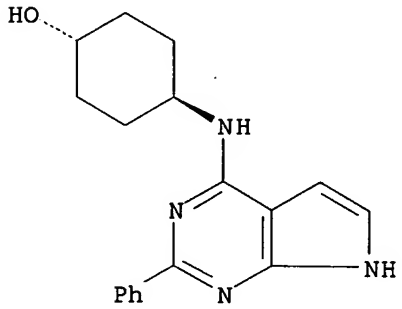
L5 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:927211 CAPLUS
DOCUMENT NUMBER: 141:384321
TITLE: Polymorphic forms of 4-(4-trans-Hydroxycyclohexyl)amino-2-phenyl-7H-pyrrolo[2,3'-d]pyrimidine hydrogen mesylate
INVENTOR(S): Heinrich, Timo; Pahl, Axel; Luitjens, Bernd-Martin; Finner, Emil; Verveer, Pieter C.; Zorgdrager, Jan
PATENT ASSIGNEE(S): Solvay Pharmaceuticals G.m.b.H., Germany
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004094428	A1	20041104	WO 2004-EP50573	20040421
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004232495	A1	20041104	AU 2004-232495	20040421
CA 2522810	AA	20041104	CA 2004-2522810	20040421
US 2004248912	A1	20041209	US 2004-828650	20040421
EP 1641797	A1	20060405	EP 2004-728571	20040421
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004009511	A	20060418	BR 2004-9511	20040421
CN 1777606	A	20060524	CN 2004-80010690	20040421
NO 2005005495	A	20060123	NO 2005-5495	20051121
PRIORITY APPLN. INFO.:			EP 2003-101093 A	20030422
			US 2003-464422P P	20030422
			WO 2004-EP50573 W	20040421

IT 251945-92-3
RL: PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(polymorphic forms of (hydroxycyclohexyl)aminopyrrolopyrimidine hydrogen mesylate)
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



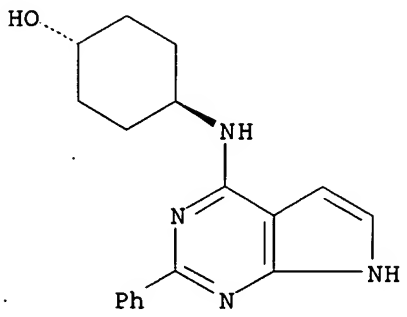
IT 685561-51-7P
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(polymorphic forms of (hydroxycyclohexyl)aminopyrrolopyrimidine hydrogen mesylate)
RN 685561-51-7 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 251945-92-3

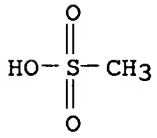
CMF C18 H20 N4 O

Relative stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S



AB The present invention relates to 4-(4-trans-hydroxycyclohexyl)amino-2-phenyl-7H-pyrrolo[2,3'-d]pyrimidine hydrogen mesylate (I), the polymorphic α and β forms and a method for the production of the compds. The polymorphic form α of I was prepared by the reaction of the corresponding base with methanesulfonic acid in MeOH. The solubility of the polymorphic forms was determined

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:88297 CAPLUS
DOCUMENT NUMBER: 140:146159
TITLE: Preparation and use of substituted pyrrolo[2,3-d]pyrimidines as selective adenosine A3 receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA
SOURCE: U.S., 71 pp., Cont.-in-part of Appl. No. PCT/US99/12135.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6686366	B1	20040203	US 1999-454075	19991202
WO 9962518	A1	19991209	WO 1999-US12135	19990601

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,

JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

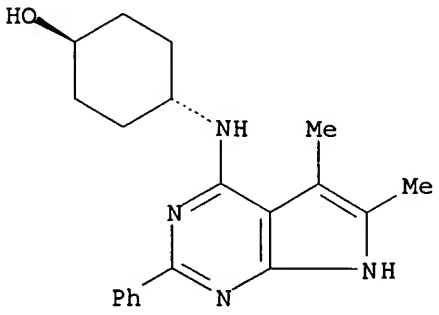
CA 2393179 AA 20010607 CA 2000-2393179 20001201
WO 2001039777 A1 20010607 WO 2000-US32702 20001201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
EP 1246623 A1 20021009 EP 2000-988011 20001201
EP 1246623 B1 20060809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2003519102 T2 20030617 JP 2001-541509 20001201
AU 784878 B2 20060713 AU 2001-24270 20001201

PRIORITY APPLN. INFO.:
US 1998-87702P P 19980602
US 1999-123216P P 19990308
US 1999-126527P P 19990326
WO 1999-US12135 A2 19990601
US 1999-454074 A 19991202
US 1999-454075 A 19991202
US 1999-454254 A 19991202
WO 2000-US32702 W 20001201

OTHER SOURCE(S): MARPAT 140:146159
IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251945-99-0P 251946-00-6P
251946-01-7P 251946-03-9P 251946-04-0P
251946-05-1P 251946-20-0P 251946-57-3P
251946-58-4P 343632-03-1P 343632-05-3P
343632-07-5P 343632-67-7P 343969-79-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A3 receptor antagonists)

RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

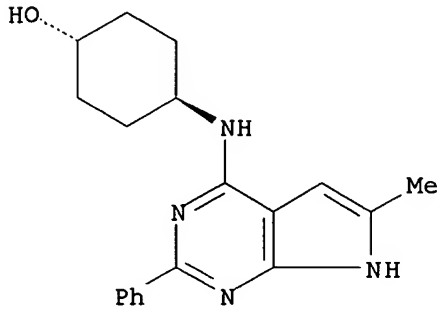
Relative stereochemistry.



RN 251945-90-1 CAPLUS

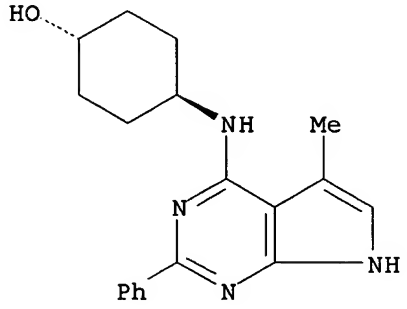
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



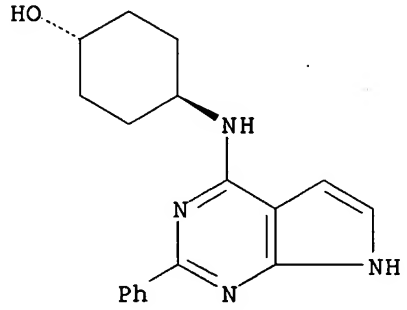
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



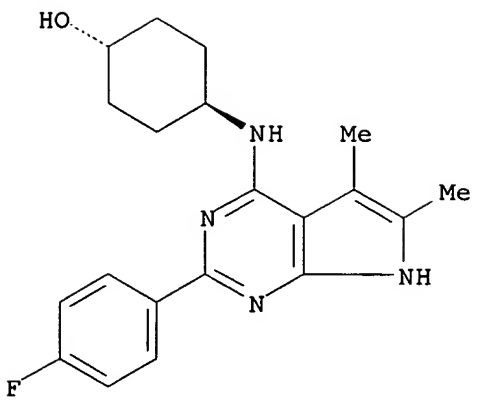
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



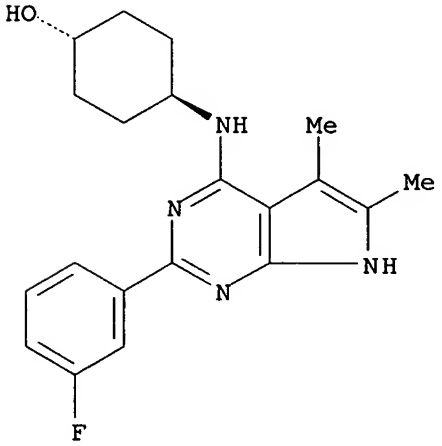
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



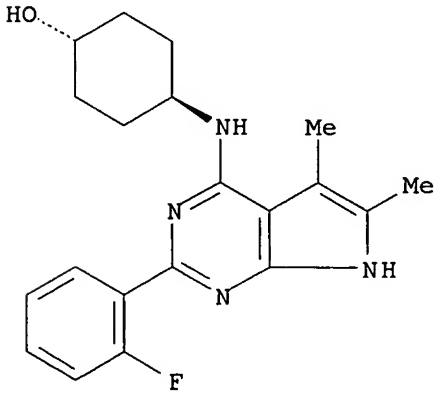
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



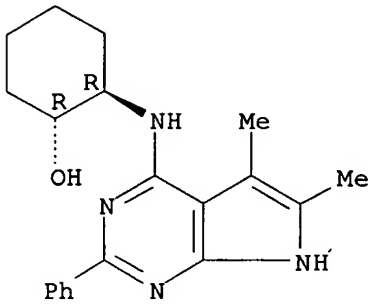
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



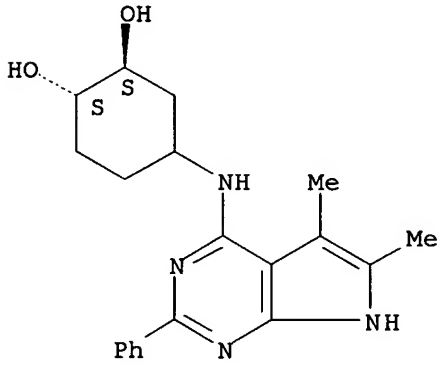
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



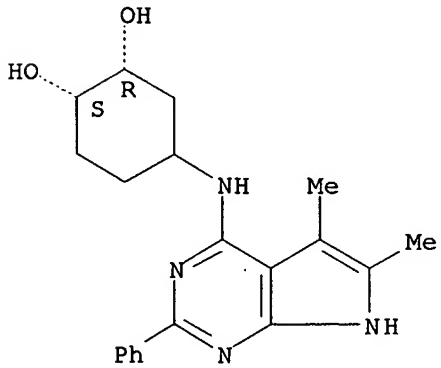
RN 251946-04-0 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-05-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

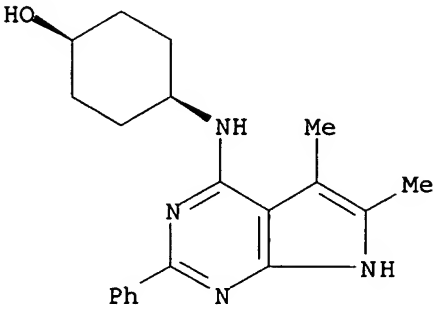
Relative stereochemistry.



RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-

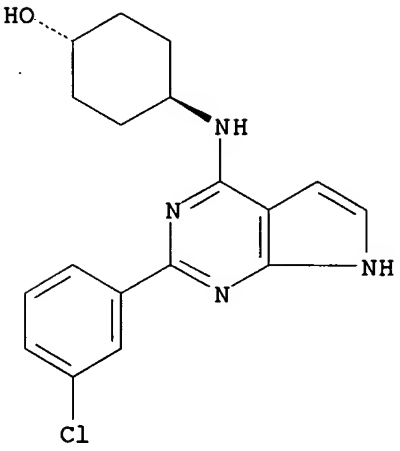
yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



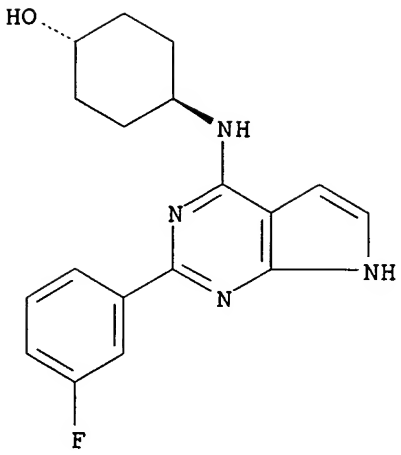
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



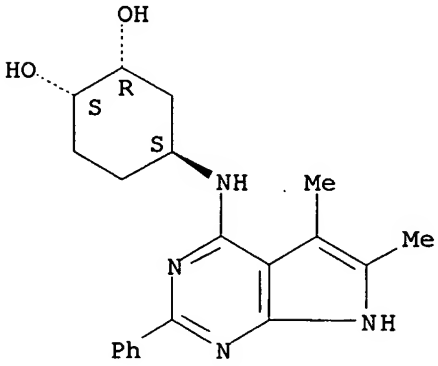
RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



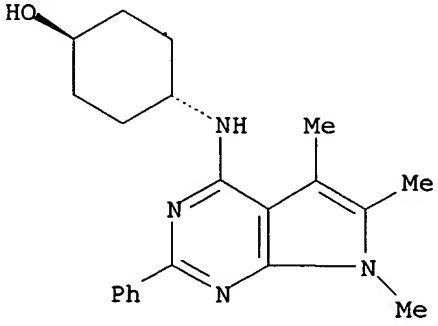
RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



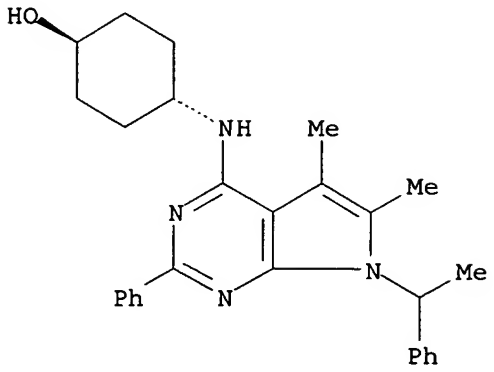
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



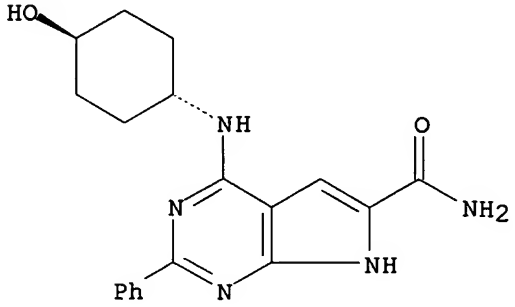
RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



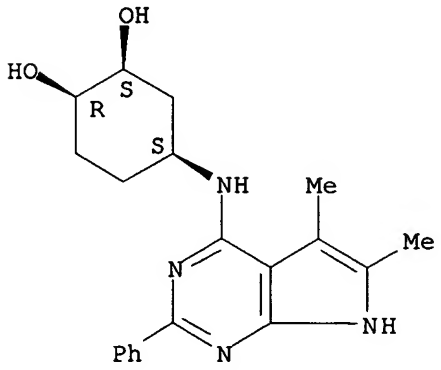
RN 343632-67-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxamide, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

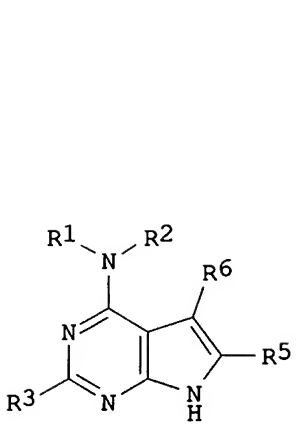


RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) . (CA INDEX NAME)

Relative stereochemistry.



GI



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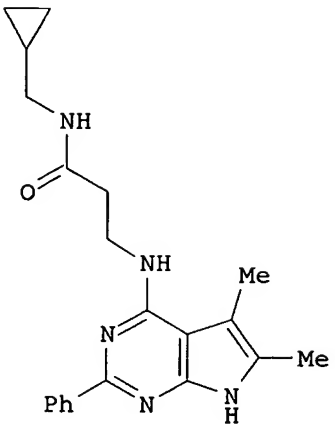


II

AB The title compds. [I; R1 = H and R2 = cyclopropylmethylaminocarbonylethyl, cis-3-hydroxycyclopentyl, acetamidobutyl, etc.; or NR1R2 = 3-acetamidopiperadino, 3-hydroxypyrrolidino, 3-methoxycarbonylmethylpyrrolidino, etc.; R3 = (un)substituted cycloalkyl, aryl; R5 = H, alkyl, aryl; R6 = H, alkyl, cycloalkyl] which specifically inhibit the adenosine A3 receptor and are useful for treating a disease associated with A3 adenosine receptor, were prepared Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was reacted with 4-trans-hydroxycyclohexylamine in DMSO at 130°C for 5 h to yield I [R1 = H; R2 = trans-4-hydroxycyclohexyl; R3 = Ph; R5, R6 = Me] in 75% yield after purification which showed Ki of 13.9 nM against adenosine receptor A1 binding. Some of the compds. I such as II exhibited at least 10 times more selective binding to adenosine receptor A3 than other receptor subtype. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease associated with A3 adenosine receptors in a subject.

REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:570644 CAPLUS
DOCUMENT NUMBER: 139:133575
TITLE: Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan
PATENT ASSIGNEE(S): OSI Pharmaceuticals Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 105 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

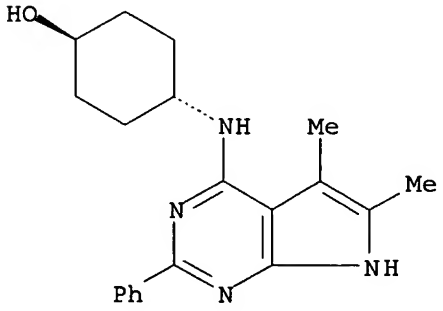
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003139427	A1	20030724	US 2002-227378	20020823
PRIORITY APPLN. INFO.:			US 2002-227378	20020823

OTHER SOURCE(S): MARPAT 139:133575
IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251945-99-0P 251946-00-6P
251946-01-7P 251946-03-9P 251946-20-0P
251946-57-3P 251946-58-4P 343632-01-9P
343632-02-0P 343632-03-1P 343632-05-3P

343632-07-5P 343969-79-9P 443118-43-2P
443118-44-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)

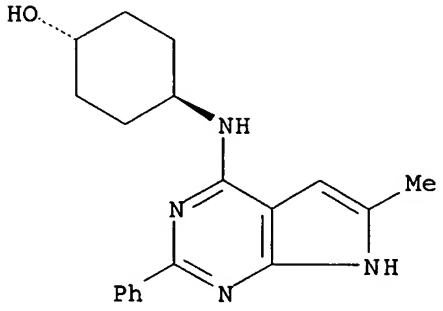
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



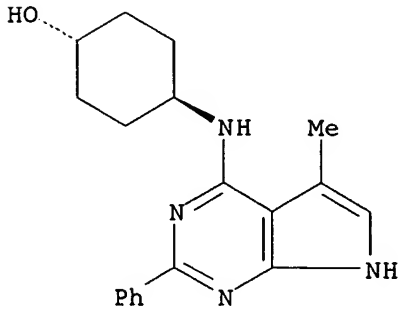
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



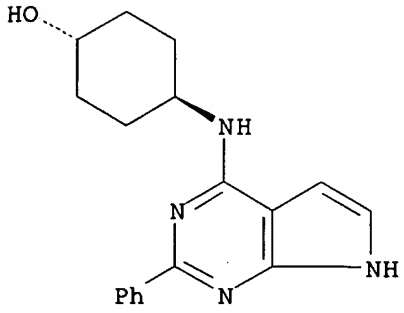
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



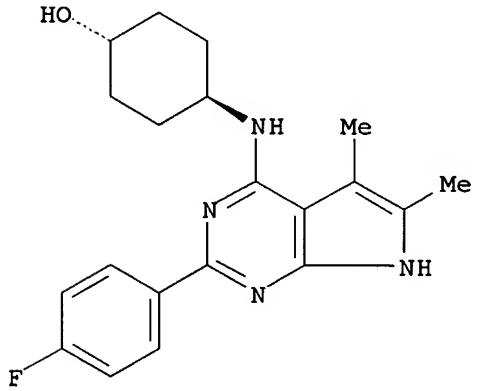
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



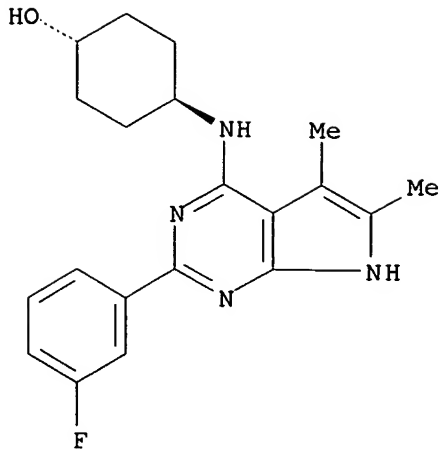
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



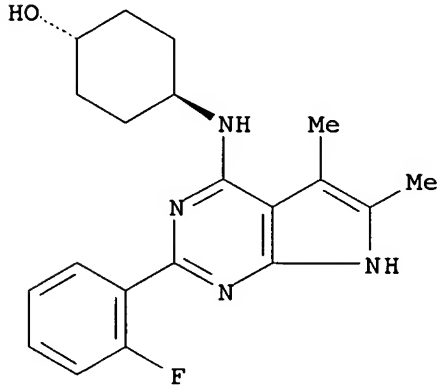
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



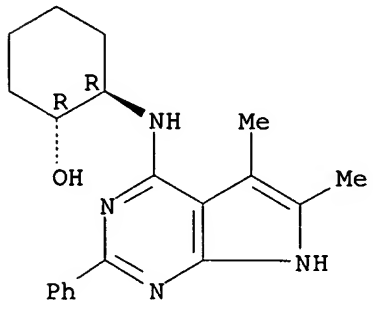
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



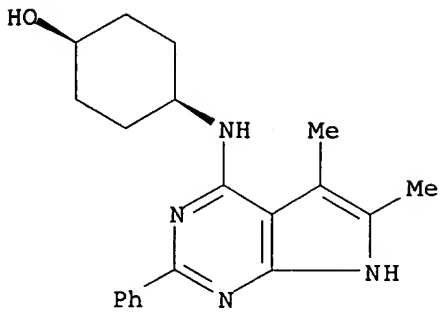
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



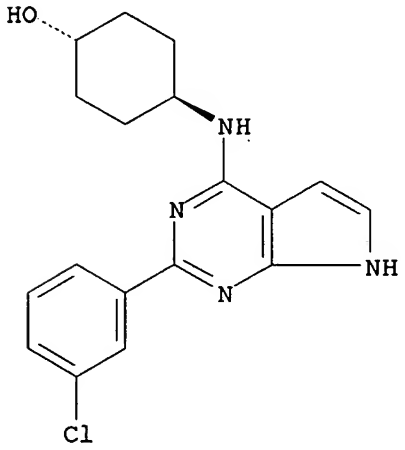
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



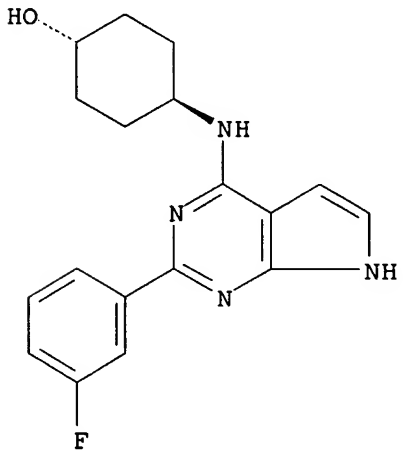
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



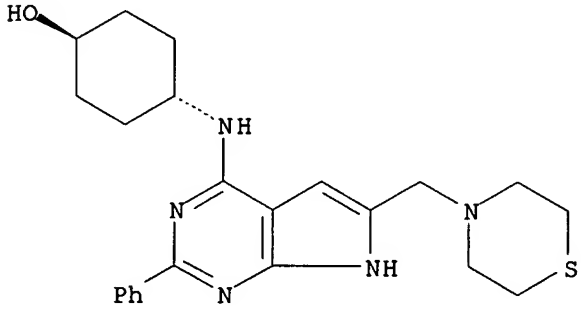
RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



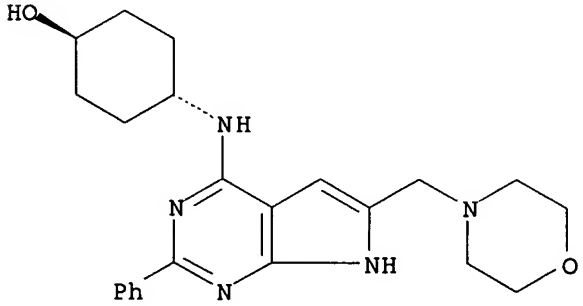
RN 343632-01-9 CAPLUS
CN Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



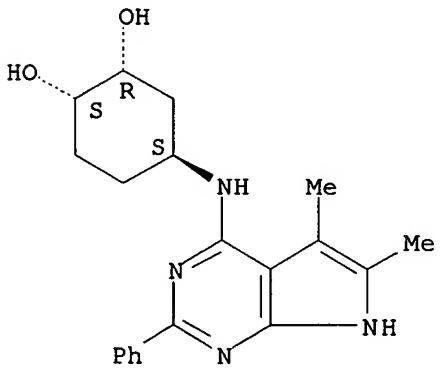
RN 343632-02-0 CAPLUS
CN Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



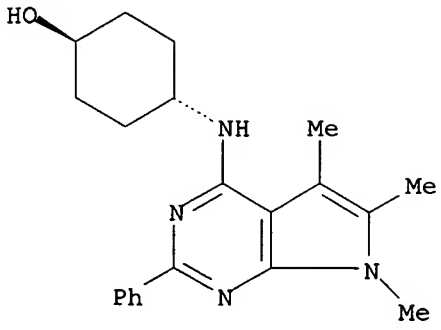
RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



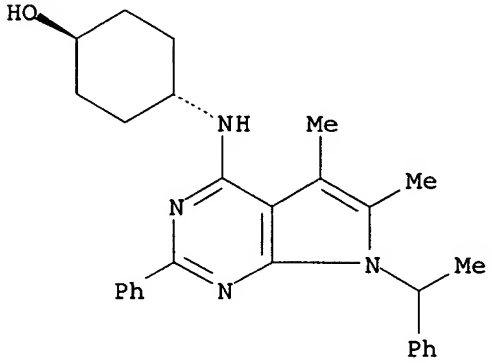
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



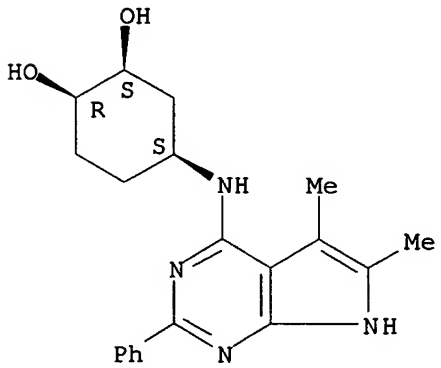
RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



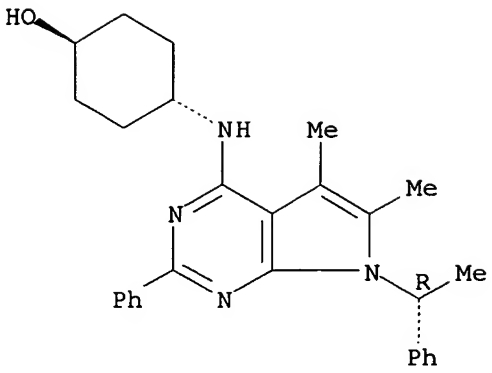
RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



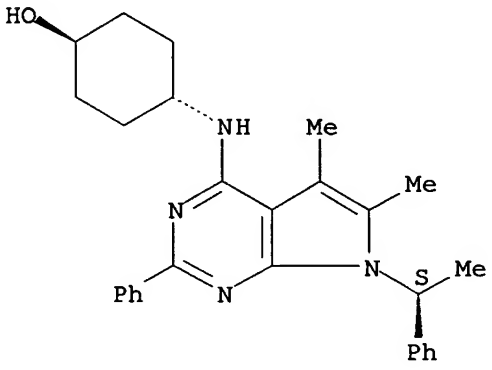
RN 443118-43-2 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

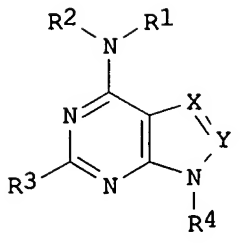


RN 443118-44-3 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-[(1S)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



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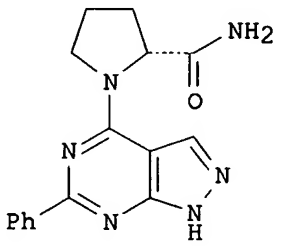


II

AB Title compds. I [Y = N, CR5 and X = N, CR6 wherein X, Y are both N or when Y = CR5, X = N or when X = CR6, Y = N; R1-2 = H, alkoxy, aminoalkyl, etc; R3-4 = H, alkyl, aryl, alkylaryl] are prepared For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 50°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, K2CO3, 100°, 16 h), converted to the chloride (POCl3, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has Ki = 76.7 nM for the adenosine A1 receptor, Ki = 242.7 nM for A2a and Ki = 1480.5 nM for A2b. I are useful

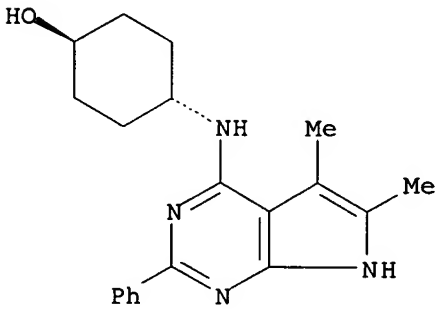
for the treatment of.

L5 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:300617 CAPLUS
DOCUMENT NUMBER: 138:321287
TITLE: Preparation of deazapurines as adenosine A3 receptor antagonists.
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 77 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073708	A1	20030417	US 2001-6405	20011130
US 6673802	B2	20040106		
PRIORITY APPLN. INFO.:			US 2000-250748P P	20001201

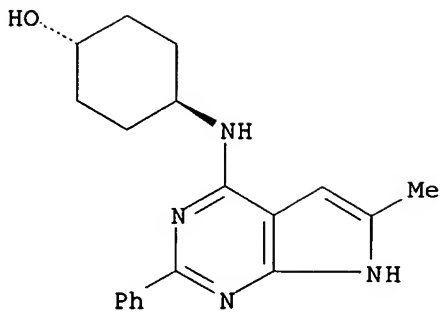
OTHER SOURCE(S): MARPAT 138:321287
IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251945-99-0P 251946-00-6P
251946-01-7P 251946-04-0P 251946-05-1P
251946-20-0P 251946-57-3P 251946-58-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of deazapurines as adenosine A3 receptor antagonists)
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



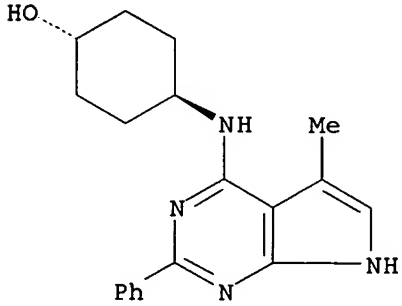
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



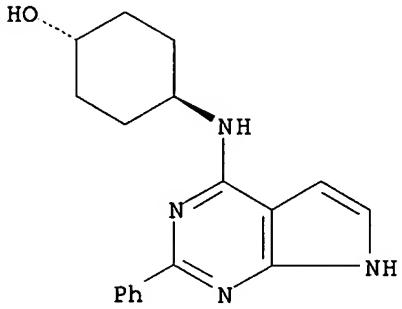
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



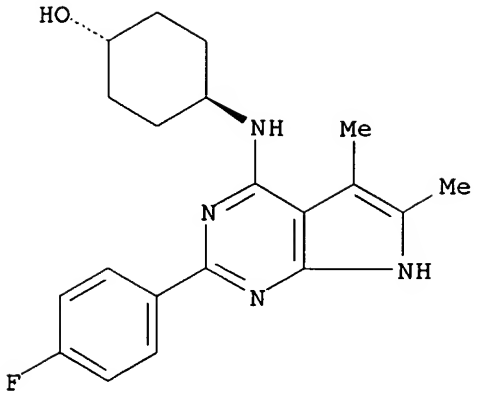
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



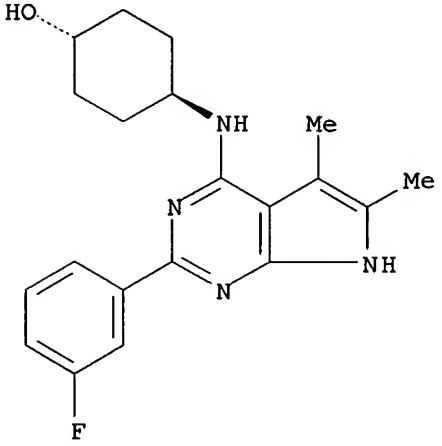
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



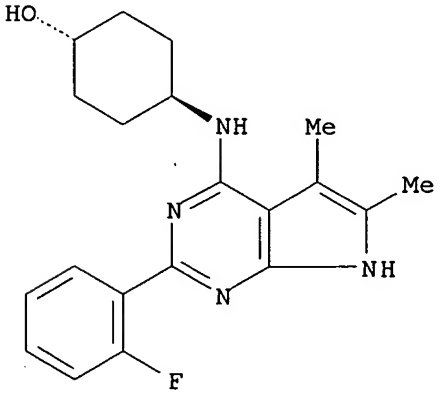
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



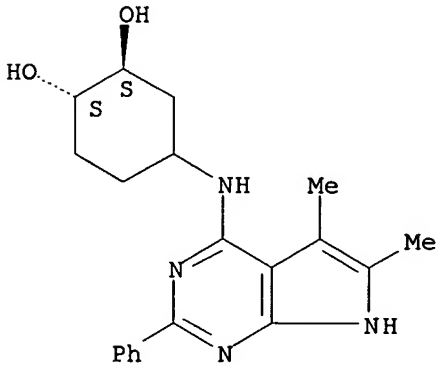
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



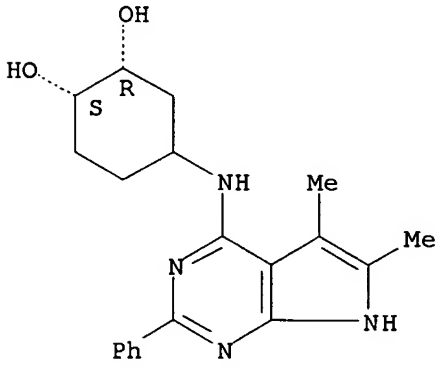
RN 251946-04-0 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



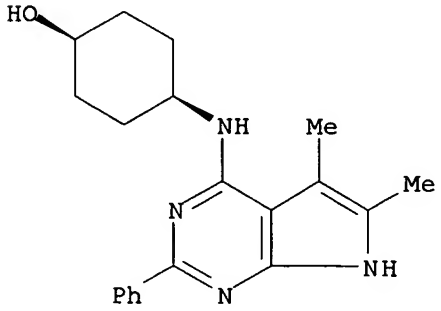
RN 251946-05-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

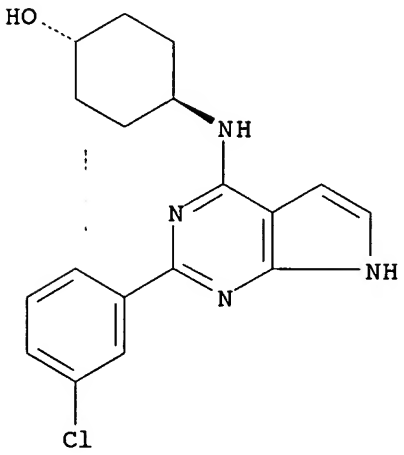
Relative stereochemistry.



RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-

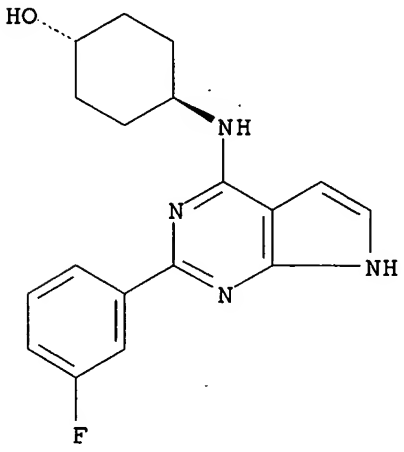
yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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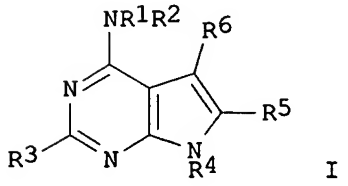


I

AB Title compds. [I; R1, R2 = H, (substituted) alkyl, aryl, aralkyl; R1R2 = atoms to form (substituted) heterocyclyl; R3 = (substituted) alkyl, aryl, aralkyl; R4 = H, (substituted) alkyl, aryl, aralkyl; R5, R6 = H, halo,

(substituted) alkyl, aryl, alkylaryl; R4R5 or R5R6 = (substituted) heterocyclyl, carbocyclyl], were prepared Thus, 2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamine and histamine were heated at 120° in Me2SO for 6.5 h to give 43% [2-(3H-imidazol-4-yl)ethyl] [2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amine. The latter had 10 times the A3 receptor binding affinity of a reference compound

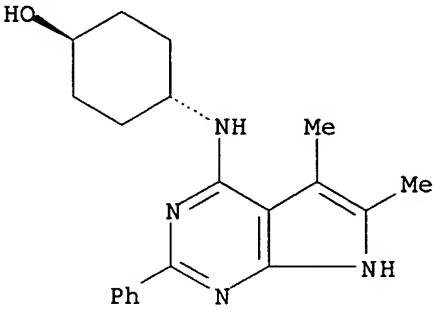
REFERENCE COUNT: 118 THERE ARE 118 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:174478 CAPLUS
DOCUMENT NUMBER: 138:221598
TITLE: Preparation of pyrrolo[2,3-d]pyrimidinamines as selective adenosine A1 receptor inhibitors for treatment of asthma, COPD, and other conditions
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 79 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2003045536	A1	20030306	US 2001-280		20011130
US 6680324	B2	20040120			
US 2004082598	A1	20040429	US 2003-718280		20031120
US 2004082599	A1	20040429	US 2003-718411		20031120
PRIORITY APPLN. INFO.:			US 2000-250895P	P	20001201
			US 2001-280	A1	20011130

OTHER SOURCE(S): MARPAT 138:221598
IT 246855-41-4P, 4-[(4-trans-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine 343632-64-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(A1 receptor inhibitor; preparation of pyrrolopyrimidinamines adenosine A1 receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

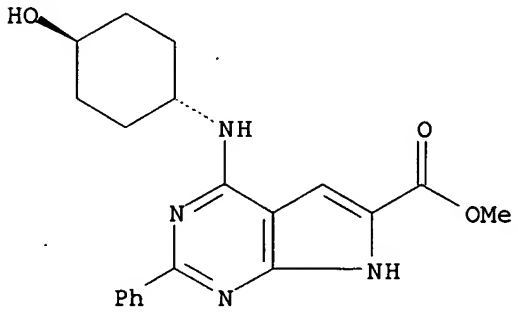
Relative stereochemistry.



RN 343632-64-4 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

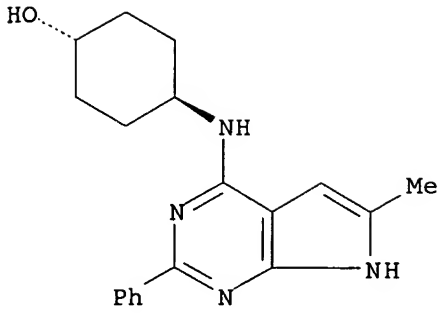


IT 251945-90-1P, 4-[(4-trans-Hydroxycyclohexyl)amino]-6-methyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine 251945-91-2P, 4-[(4-trans-Hydroxycyclohexyl)amino]-5-methyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine 251945-92-3P, 4-[(4-trans-Hydroxycyclohexyl)amino]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine 251945-99-0P, 4-[(4-trans-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(4-fluorophenyl)-7H-pyrrolo[2,3-d]pyrimidine 251946-00-6P, 4-[(4-trans-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-fluorophenyl)-7H-pyrrolo[2,3-d]pyrimidine 251946-01-7P, 4-[(4-trans-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-fluorophenyl)-7H-pyrrolo[2,3-d]pyrimidine 251946-03-9P 251946-20-0P, 4-[(4-cis-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine 251946-57-3P, 4-[(trans-4-Hydroxycyclohexyl)amino]-2-(3-chlorophenyl)-7H-pyrrolo[2,3-d]pyrimidine 251946-58-4P, 4-[(trans-4-Hydroxycyclohexyl)amino]-2-(3-fluorophenyl)-7H-pyrrolo[2,3-d]pyrimidine 343632-01-9P 343632-02-0P 343632-03-1P 343632-05-3P 343632-07-5P 343632-61-1P, trans-4-[[6-[(Imidazol-1-yl)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]cyclohexanol 343632-62-2P, trans-4-(4-Hydroxycyclohexylamino)-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid 343632-63-3P, trans-4-[[6-[(2-Hydroxyethoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]cyclohexanol 343632-67-7P, trans-4-[(4-Hydroxycyclohexyl)amino]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid amide 343969-79-9P 443118-43-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(A1 receptor inhibitor; preparation of pyrrolopyrimidinamines adenosine A1 receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

RN 251945-90-1 CAPLUS

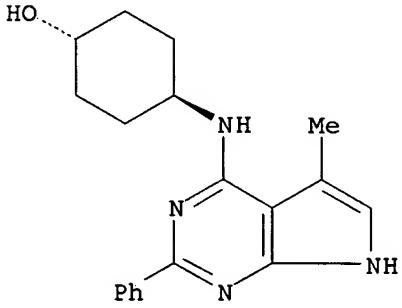
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



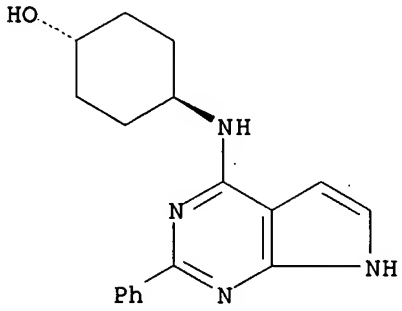
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



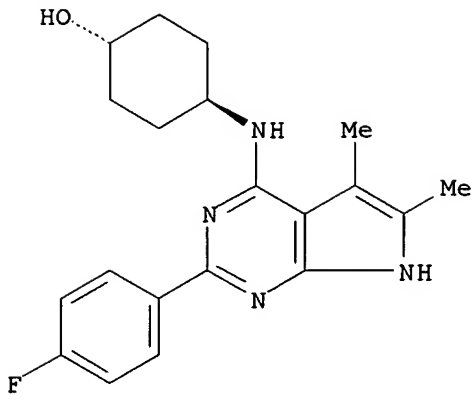
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



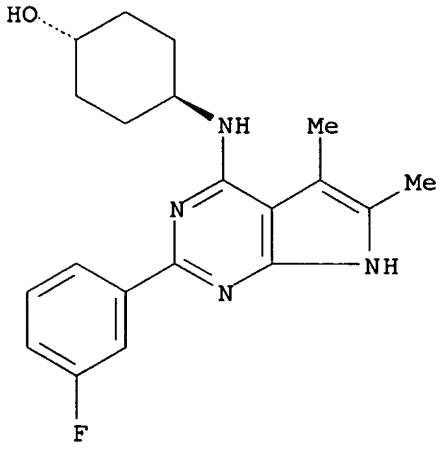
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



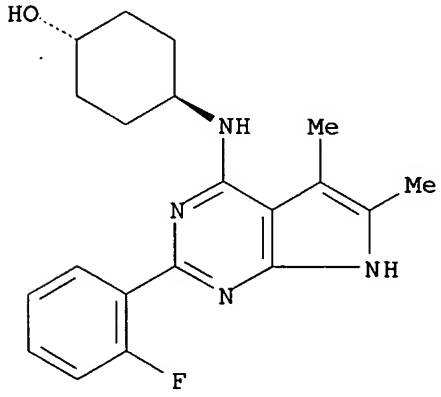
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



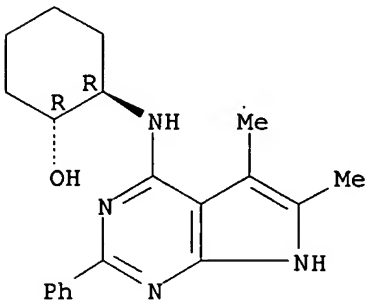
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



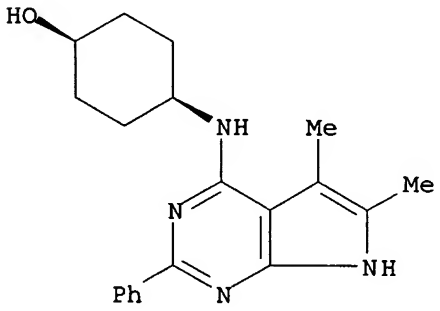
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



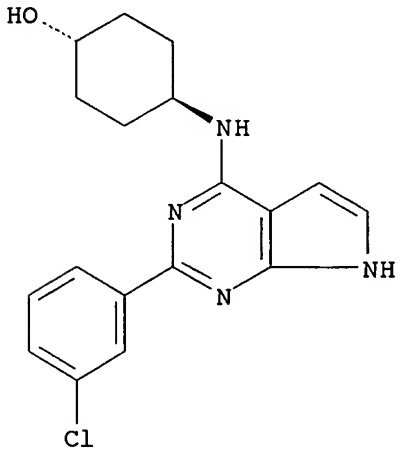
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

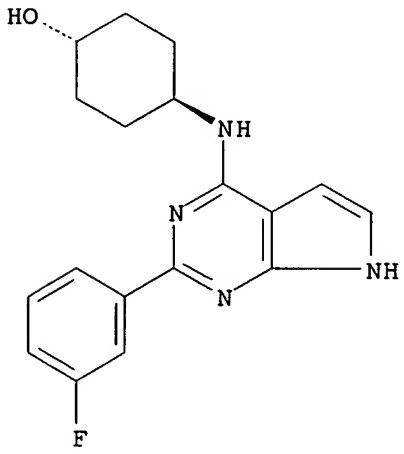
Relative stereochemistry.



RN 251946-58-4 CAPLUS

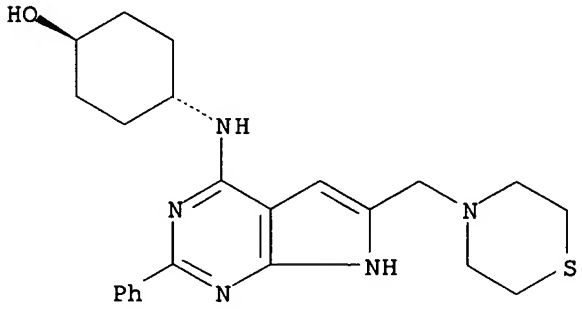
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



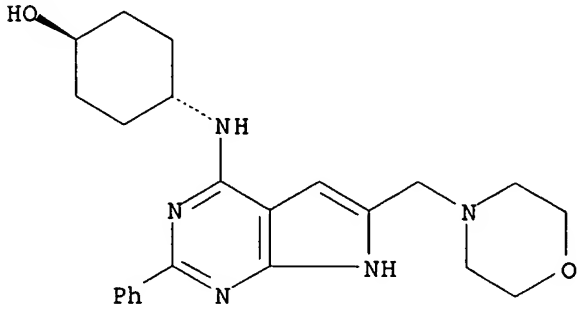
RN 343632-01-9 CAPLUS
CN Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 343632-02-0 CAPLUS
CN Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

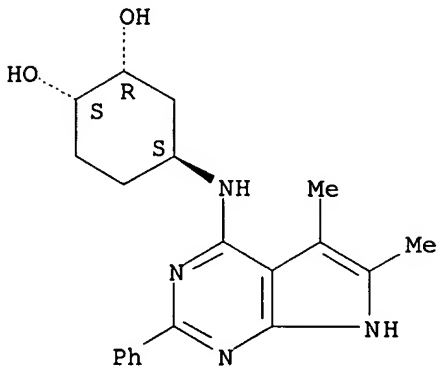
Relative stereochemistry.



RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-

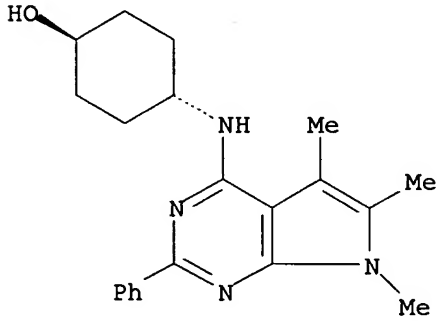
4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



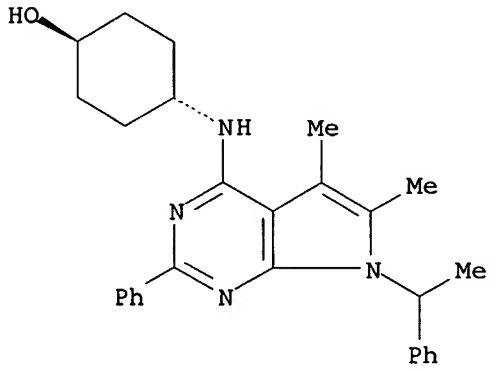
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



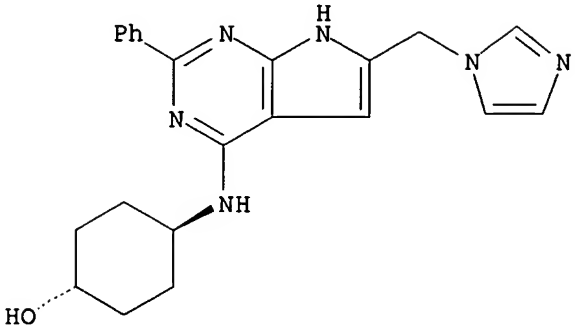
RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



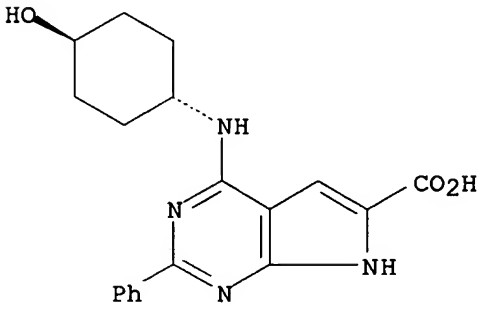
RN 343632-61-1 CAPLUS
CN Cyclohexanol, 4-[[6-(1H-imidazol-1-ylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



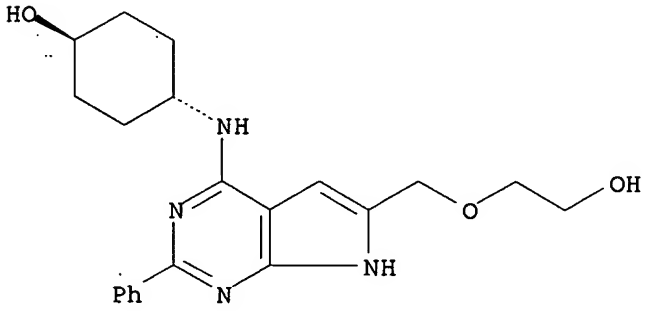
RN 343632-62-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



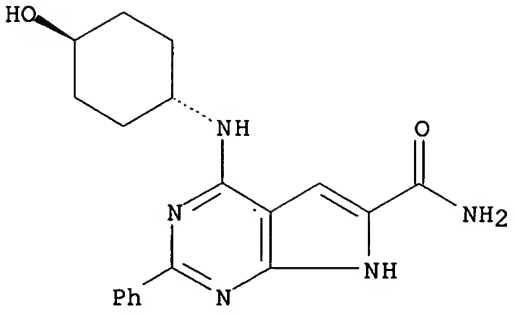
RN 343632-63-3 CAPLUS
CN Cyclohexanol, 4-[[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



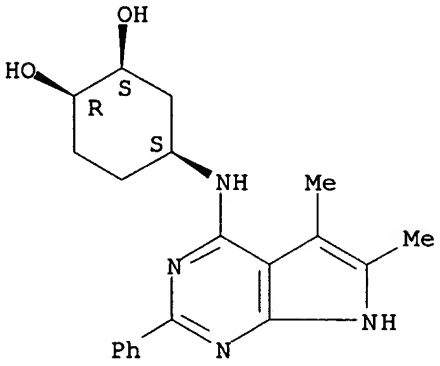
RN 343632-67-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxamide, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



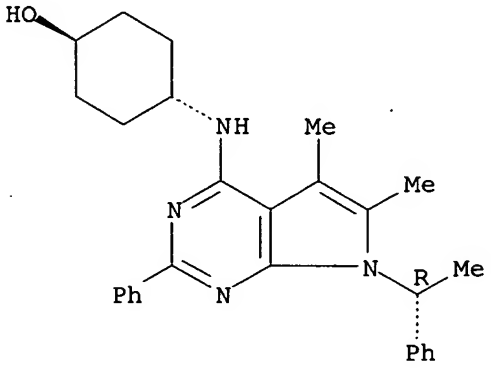
RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

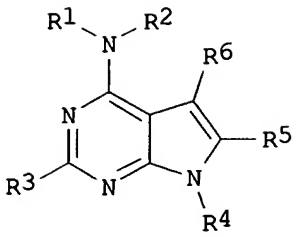


RN 443118-43-2 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



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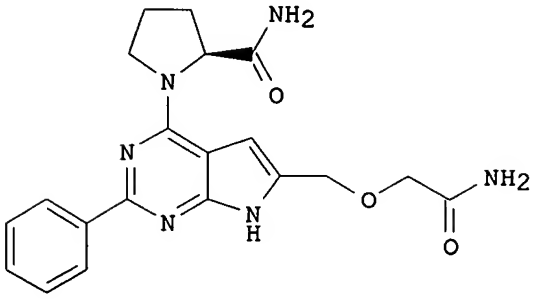

II

AB Title diazapurinamines I [wherein R1, R2, and R4 = independently H or (un)substituted alkyl(aryl) or aryl; or NR1R2 = (un)substituted heterocyclyl; R3 = (un)substituted alkyl(aryl), aryl, CO2H, carboxy esters, or carboxamides; or C2R3R4 or C2R5R6 = (un)substituted carbocyclyl or heterocyclyl; R5 and R6 = independently H, halo, or (un)substituted alkyl(aryl) or aryl; and pharmaceutically acceptable salts and prodrugs thereof] were prepared as adenosine A1 specific inhibitors. For example, 4-chloro-5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidine was protected with di-t-Bu dicarbonate (80%), brominated (84%), coupled with anhydrous Me glycolate (99%), coupled with L-prolinamide (92%), and deprotected (93%) to give II. The latter exhibited adenosine A1 receptor binding equal to or surpassing that of reference compds. and is expected to have better water solubility (cLogP = 1.5) than reference compds. (cLogP = 3.8). Efficacy and structure activity profiles of diazapurines of the invention are also disclosed. Thus, I are useful for the treatment of asthma, chronic obstructive pulmonary disease (COPD), allergic rhinitis, upper respiratory disorder, and congestive heart failure (no data).

L5 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:555495 CAPLUS
DOCUMENT NUMBER: 137:109485
TITLE: Preparation of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 320 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057267	A1	20020725	WO 2001-US45280	20011130

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002058667	A1	20020516	US 2000-728316	20001201
US 6680322	B2	20040120		
US 2002094974	A1	20020718	US 2000-728616	20001201
US 2003036545	A1	20030220	US 2000-728607	20001201
US 6664252	B2	20031216		
CA 2430577	AA	20020725	CA 2001-2430577	20011130
EP 1347980	A1	20031001	EP 2001-997029	20011130
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BR 2001015847	A	20040225	BR 2001-15847	20011130
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NZ 525885	A	20050128	NZ 2001-525885	20011130
NO 2003002482	A	20030728	NO 2003-2482	20030602

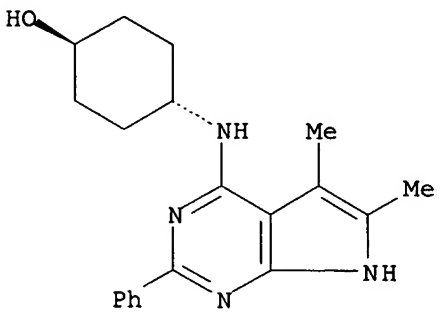
PRIORITY APPLN. INFO.:	US 1999-169037P	P 19991202
	US 2000-728316	A 20001201
	US 2000-728616	A 20001201
	US 2000-728607	A 20001204
	US 1999-168803P	P 19991202
	US 1999-169036P	P 19991202
	WO 2001-US45280	W 20011130

OTHER SOURCE(S): MARPAT 137:109485

IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251945-99-0P 251946-00-6P
251946-01-7P 251946-20-0P 251946-57-3P
251946-58-4P 343632-01-9P 343632-02-0P
343632-03-1P 343632-05-3P 343632-07-5P
343632-61-1P 343632-62-2P 343632-63-3P
343632-64-4P 343632-67-7P 343969-79-9P
443760-79-0P 443760-80-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

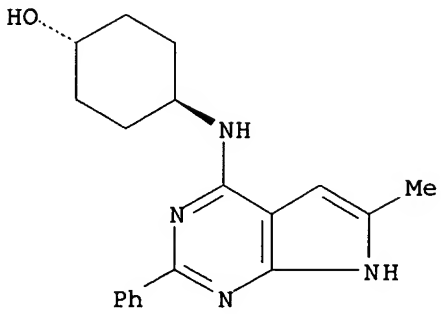
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



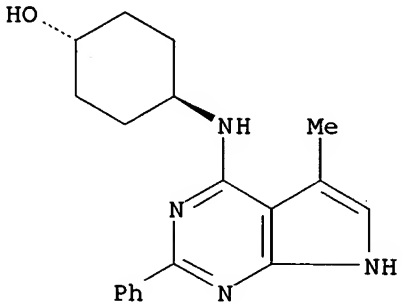
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



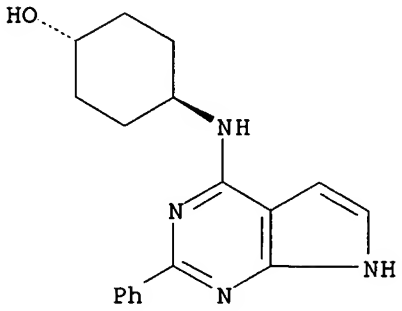
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



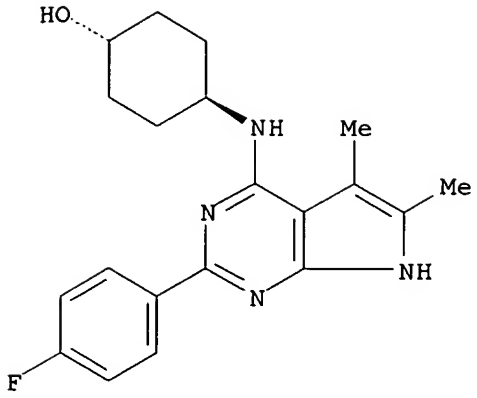
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



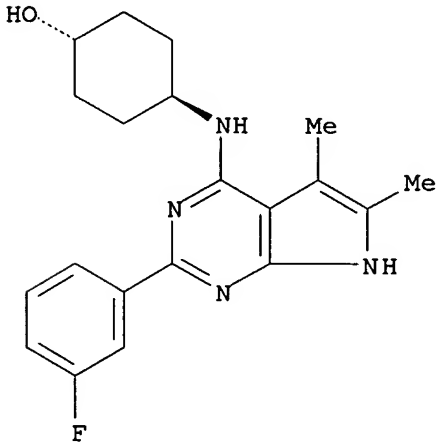
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



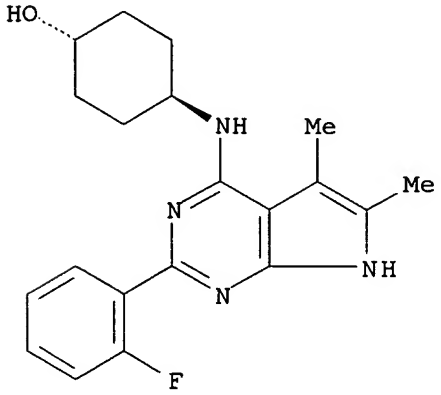
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



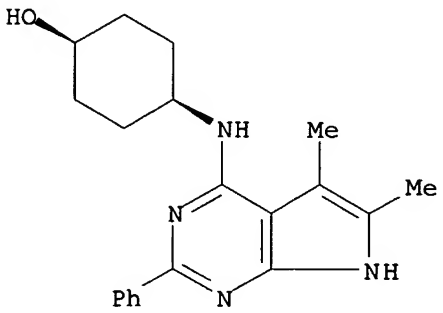
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



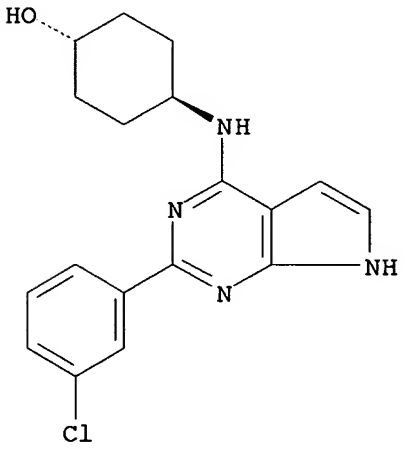
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



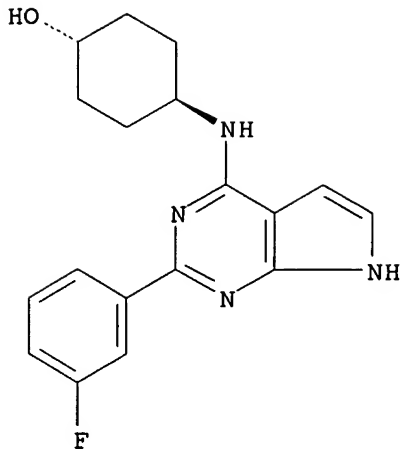
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



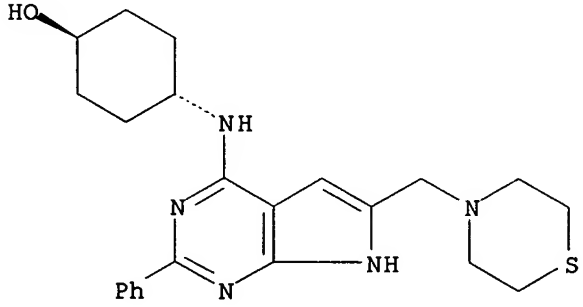
RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



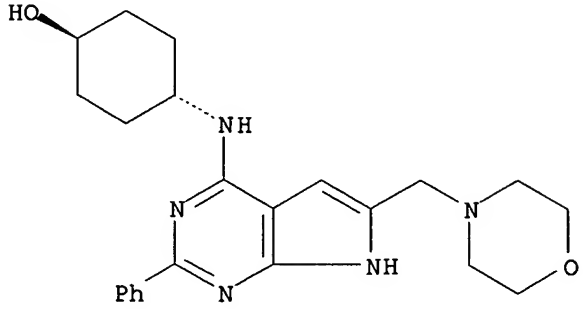
RN 343632-01-9 CAPLUS
CN Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



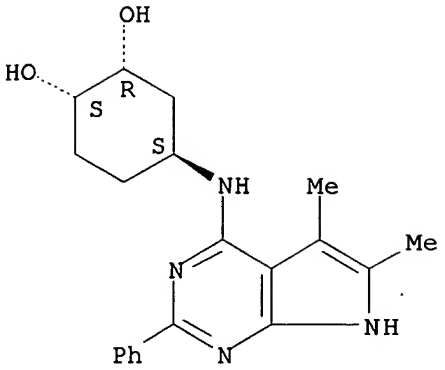
RN 343632-02-0 CAPLUS
CN Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



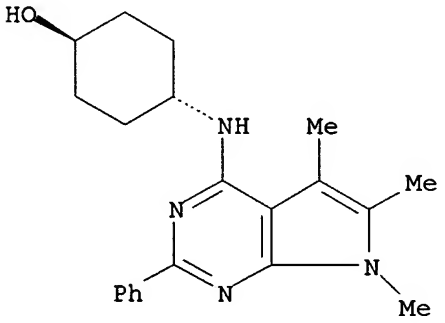
RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



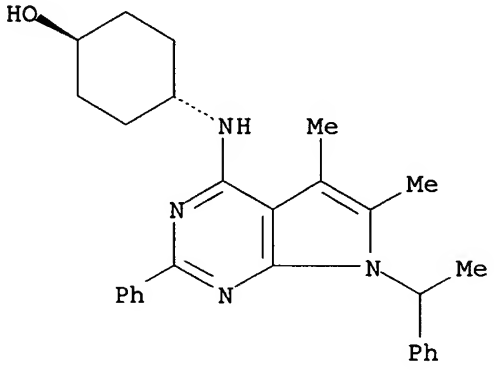
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



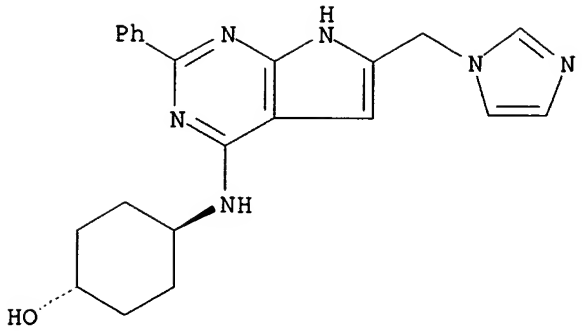
RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



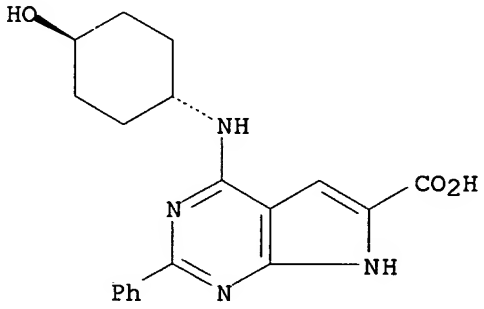
RN 343632-61-1 CAPLUS
CN Cyclohexanol, 4-[[6-(1H-imidazol-1-ylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



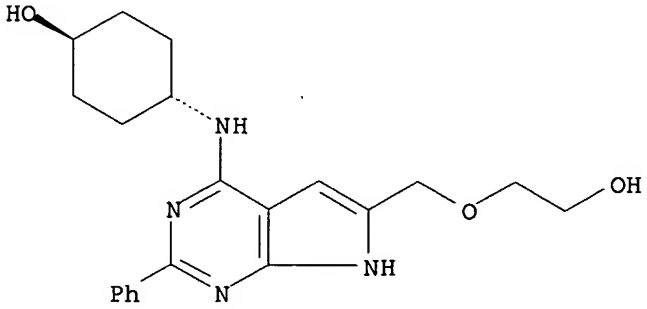
RN 343632-62-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



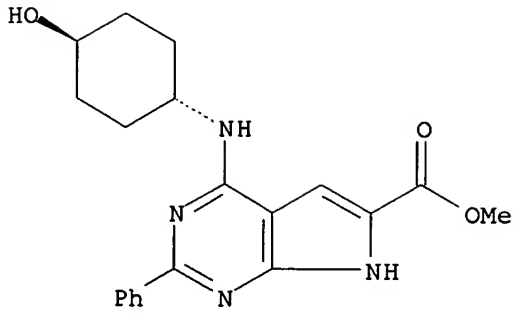
RN 343632-63-3 CAPLUS
CN Cyclohexanol, 4-[[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



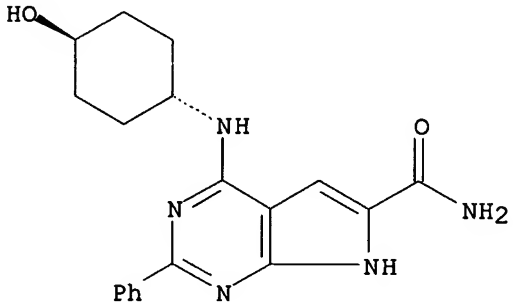
RN 343632-64-4 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



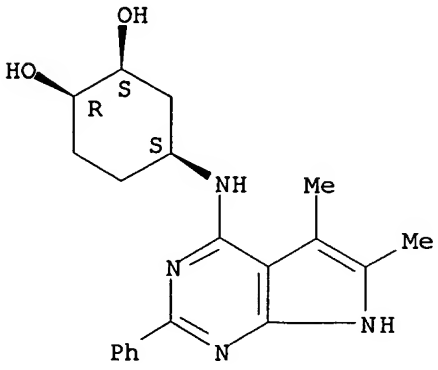
RN 343632-67-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxamide, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



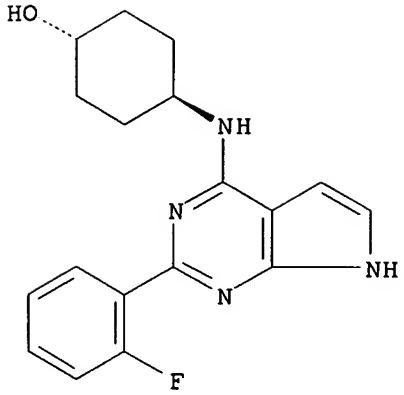
RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



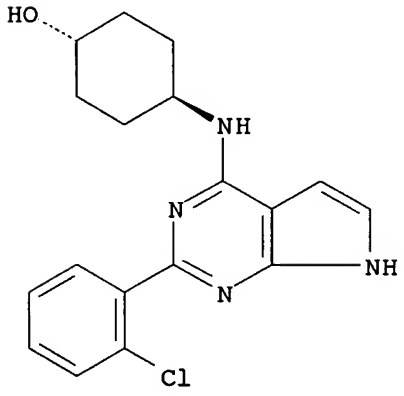
RN 443760-79-0 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 443760-80-3 CAPLUS
CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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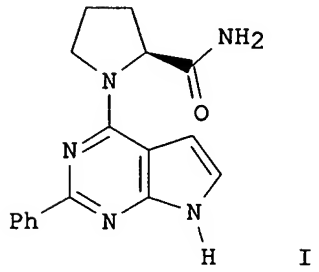

I

AB Title compds., e.g., I, were prepared Data for biol. activity of title compds. were given.
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:540257 CAPLUS

DOCUMENT NUMBER: 137:109288
TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 83 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002094974	A1	20020718	US 2000-728616	20001201
CA 2430577	AA	20020725	CA 2001-2430577	20011130
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
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EP 1347980	A1	20031001	EP 2001-997029	20011130
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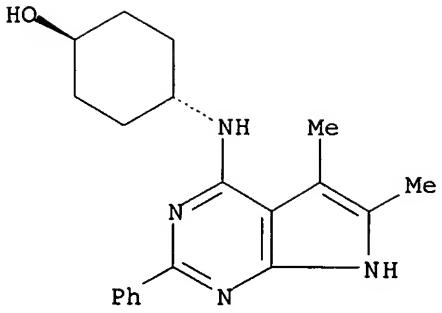
JP 2004517896	T2	20040617	JP 2002-557944	20011130
NZ 525885	A	20050128	NZ 2001-525885	20011130
NO 2003002482	A	20030728	NO 2003-2482	20030602

PRIORITY APPLN. INFO.:

US 1999-169036P	P	19991202
US 1999-169037P	P	19991202
US 2000-728316	A	20001201
US 2000-728607	A	20001201
US 2000-728616	A	20001201
WO 2001-US45280	W	20011130

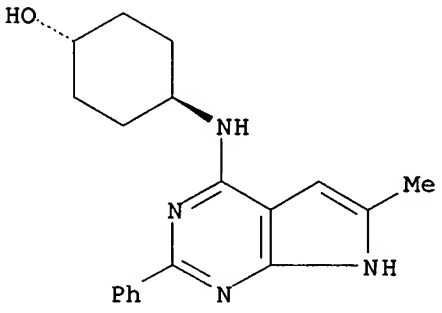
OTHER SOURCE(S): MARPAT 137:109288
IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251946-03-9P 251946-20-0P
251946-57-3P 251946-58-4P 443118-21-6P
443118-22-7P 443118-23-8P 443118-24-9P
443118-43-2P 443118-44-3P 443118-49-8P
443118-66-9P 443118-71-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(invention compound; preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



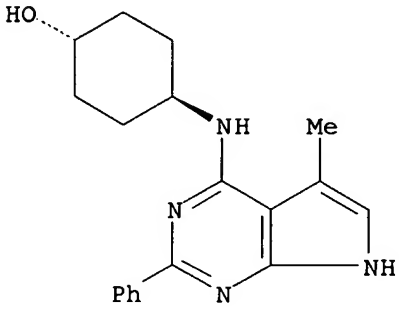
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



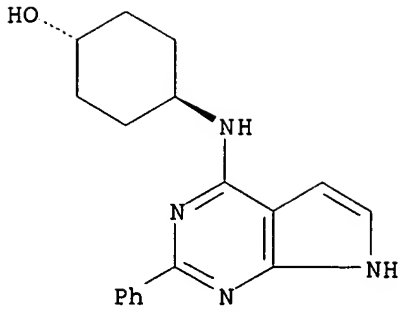
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



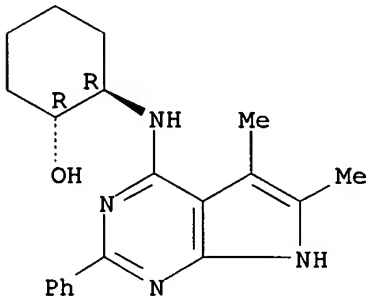
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



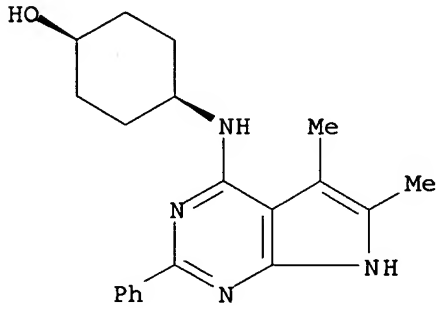
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



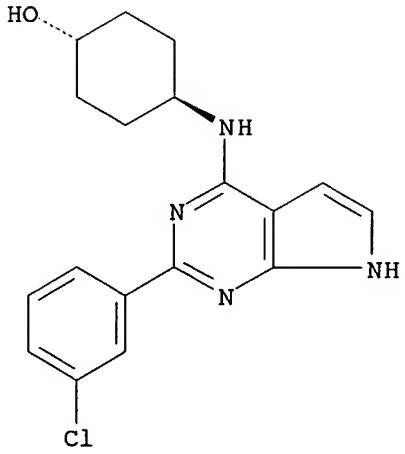
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



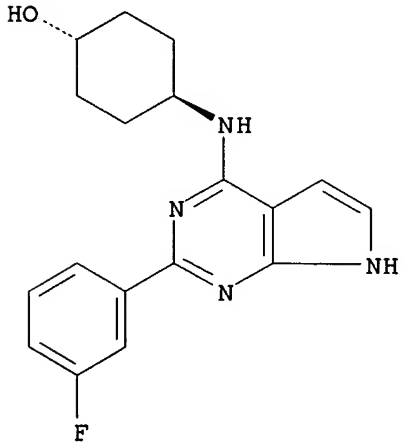
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



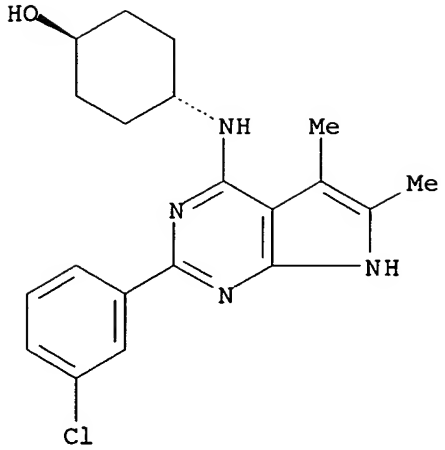
RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



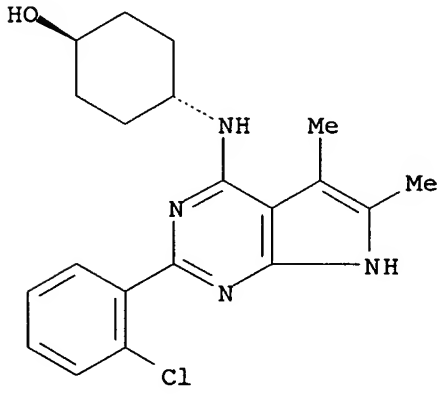
RN 443118-21-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



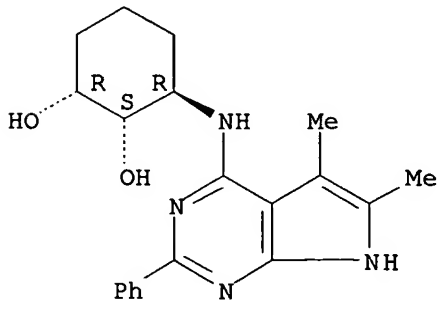
RN 443118-22-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 443118-23-8 CAPLUS
CN 1,2-Cyclohexanediol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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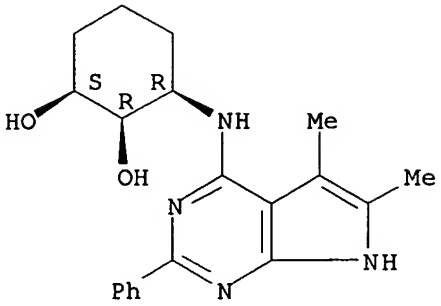
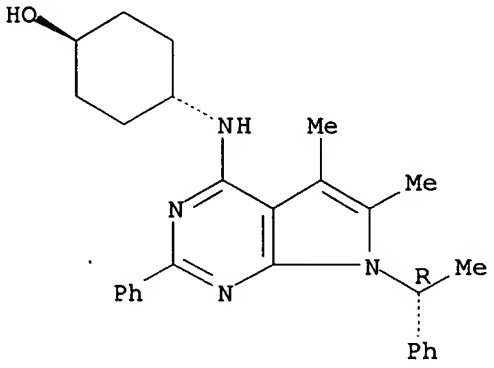
CN 1,2-Cyclohexanediol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



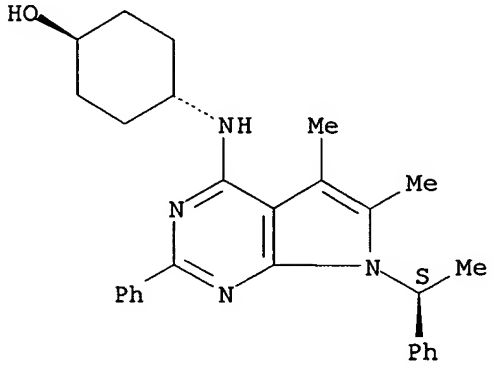
RN 443118-43-2 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-[(1R)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443118-44-3 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-[(1S)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443118-49-8 CAPLUS
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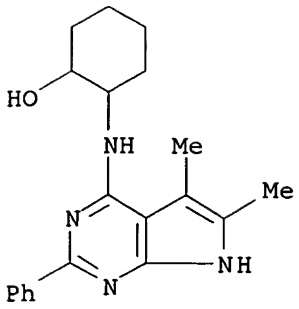
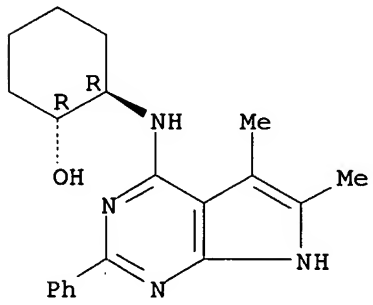


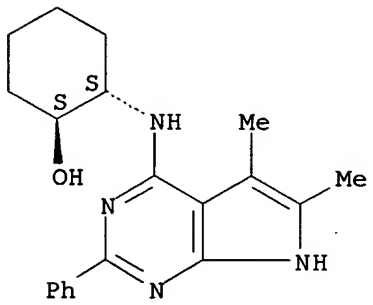
RN 443118-66-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443118-71-6 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1S,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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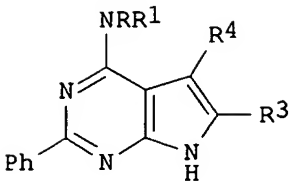

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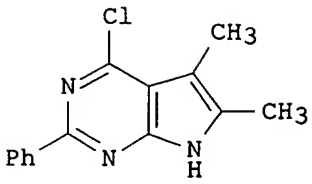

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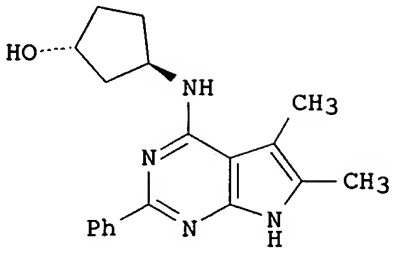

III

AB Pyrrolopyrimidines I [R = 3-hydroxycyclopentylamino ethylamino carbonylamino Pr, N,N-diethylamino carbonylamino Et, thioacetamido Et, 3-amino acetyloxy cyclopentyl, 3-hydroxycyclopentyl, 2-pyrrolyl carbonyl aminoethyl, 2-imidazolinone Et, 1-aminocarbonyl-2-methylpropyl, 1-aminocarbonyl-2-Ph Et, 3-hydroxyazetidino, 2-imidazoleethyl, acetamidoethyl, 1-(R)-phenyl-2-hydroxyethyl, N-methylaminocarbonyl pyridyl-2-methyl; R1 = H; RR1N = 3-hydroxypyrrolidino, 3-methyloxy carbonylmethyl pyrrolidino, 3-aminocarbonylmethyl pyrrolidino, 3-hydroxymethyl piperidino; R3, R4 = H, (un)substituted alkyl, aryl] are prepared as selective inhibitors of adenosine receptors, particularly the adenosine A3 receptor, for the treatment of diseases such as asthma, diarrhea, chronic obstructive pulmonary disease, allergic rhinitis, or for the treatment of eye damage caused either by disease or injury. Human adenosine receptors are transformed into yeast; the modified yeast are used to assay the invention compds. I for their adenosine receptor binding and selectivities. E.g., 1-(1-phenylethyl)-2-amino-3-cyano-4,5-dimethylpyrrole is acylated with PhCOCl to give the benzamide which undergoes cyclocondensation with concentrated H2SO4 in MeOH to give a pyrrolopyrimidinone; removal of the phenethyl group with polyphosphoric acid and chlorination of the pyrrolopyrimidinone with POCl3 gives the intermediate chloropyrrolopyrimidine II. E.g., addition of amines such as trans-3-amino-1-cyclopentanol to II in DMSO gives aminopyrrolopyrimidines such as III. III has a Ki for the adenosine A1 receptor of 29 nM and a Ki for the adenosine A3 receptor of 3.1 nM while binding to the adenosine A2a and A2b receptors with Ki values of 191 nM and 1143 nM, resp. Formulations of these compds. are claimed (no data). Methods for the preparation of I from the acylation of aminopyrroles with acyl chlorides followed by cyclocondensation and deprotection, chlorination, and substitution of the chlorine atom with an amine are claimed.

L5 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2002:368992 CAPLUS
DOCUMENT NUMBER:	136:386128
TITLE:	Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists
INVENTOR(S):	Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S):	OSI Pharmaceuticals, Inc., USA
SOURCE:	U.S. Pat. Appl. Publ., 79 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002058667	A1	20020516	US 2000-728316	20001201
US 6680322	B2	20040120		
CA 2430577	AA	20020725	CA 2001-2430577	20011130
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1347980	A1	20031001	EP 2001-997029	20011130
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BR 2001015847	A	20040225	BR 2001-15847	20011130
JP 2004517896	T2	20040617	JP 2002-557944	20011130
NZ 525885	A	20050128	NZ 2001-525885	20011130
ZA 2003003729	A	20040514	ZA 2003-3729	20030514
NO 2003002482	A	20030728	NO 2003-2482	20030602

PRIORITY APPLN. INFO.:		
US 1999-168803P	P	19991202
US 1999-169037P	P	19991202
US 2000-728316	A	20001201
US 2000-728607	A	20001201
US 2000-728616	A	20001201
WO 2001-US45280	W	20011130

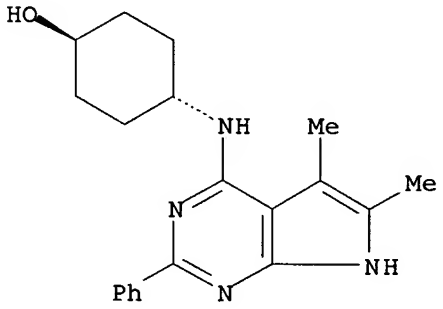
OTHER SOURCE(S): MARPAT 136:386128

IT 246855-41-4P, Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,trans 251945-90-1P, Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- 251945-91-2P, Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- 251945-92-3P, Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- 251945-99-0P, Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 251946-00-6P, Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 251946-01-7P, Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 251946-03-9P, Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,(1R,2R)-rel 251946-04-0P, 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,(1R,2R)-rel 251946-05-1P, 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,(1R,2S)-rel 251946-20-0P, Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,cis 251946-57-3P, Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 251946-58-4P, Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 343632-01-9P, Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 343632-02-0P, Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 343632-03-1P, 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,(1R,2S,4R)-rel 343632-05-3P, Cyclohexanol,

4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- 343632-07-5P, Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 343632-61-1P, Cyclohexanol, 4-[[6-(1H-imidazol-1-ylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 343632-62-2P, 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- 343632-63-3P, Cyclohexanol, 4-[[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- 343632-64-4P, 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl-, methyl ester 343632-67-7P, 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxamide, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- 343969-79-9P, 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,(1R,2S,4S)-rel
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)

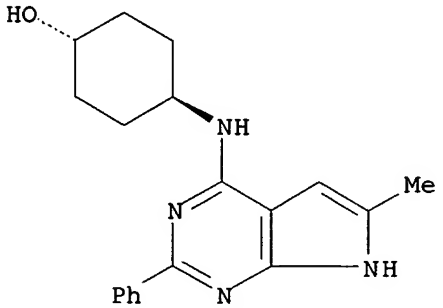
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



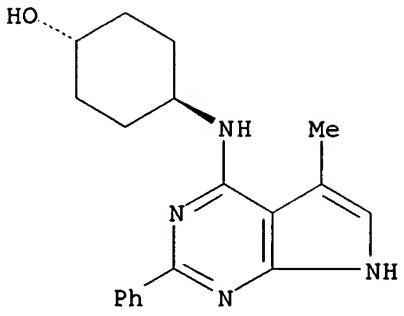
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



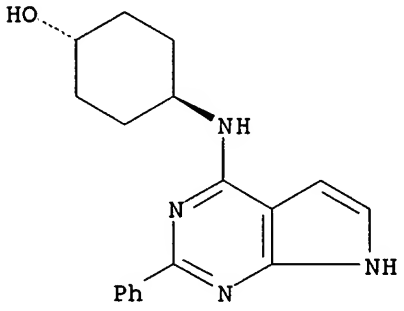
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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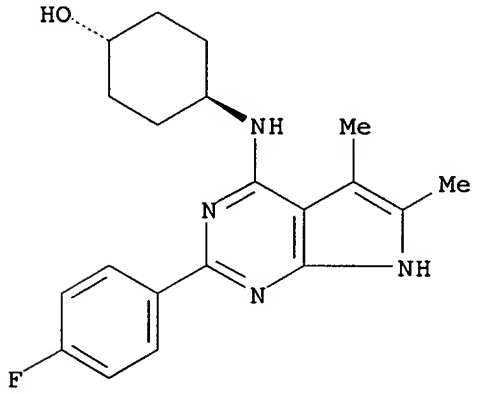
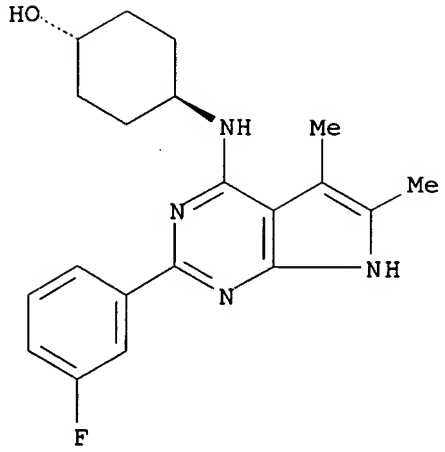
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



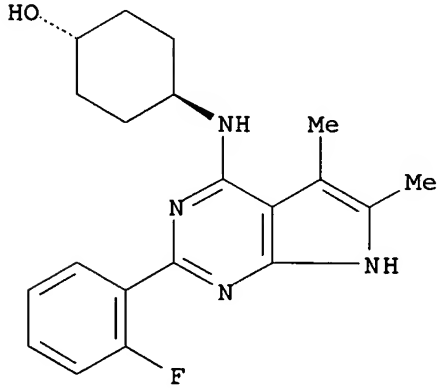
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



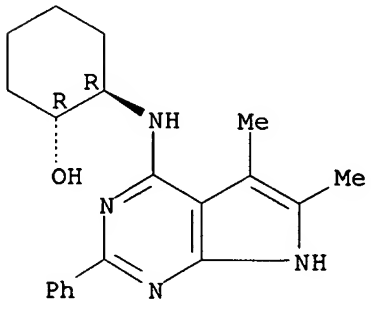
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



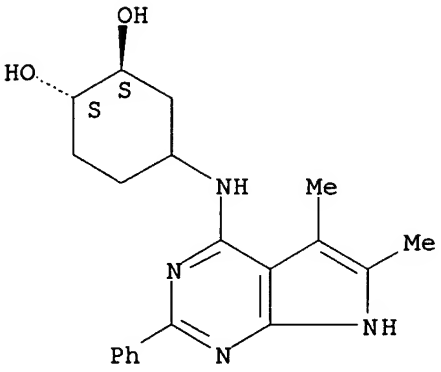
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



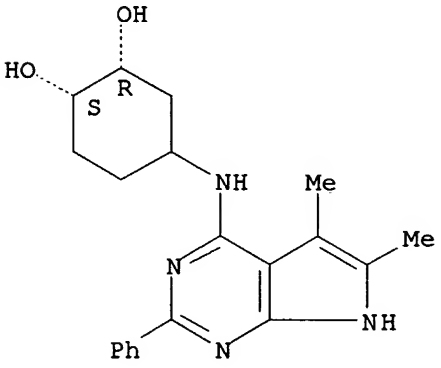
RN 251946-04-0 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



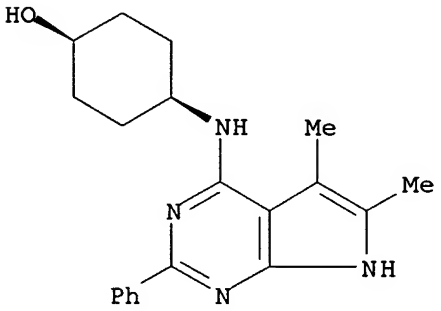
RN 251946-05-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



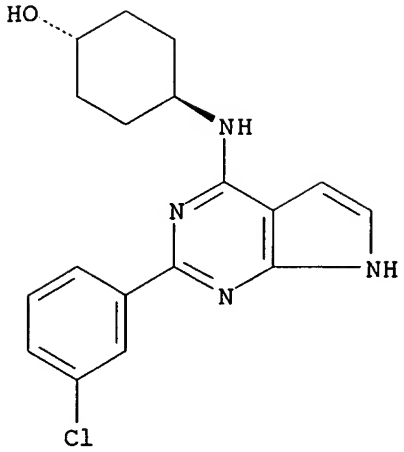
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



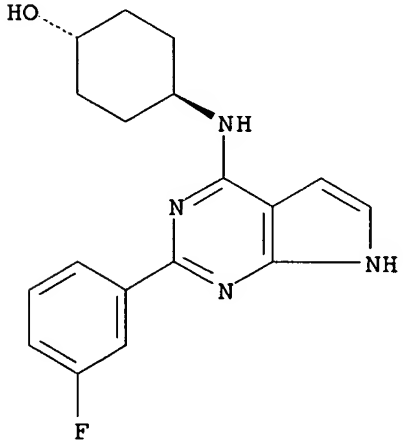
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



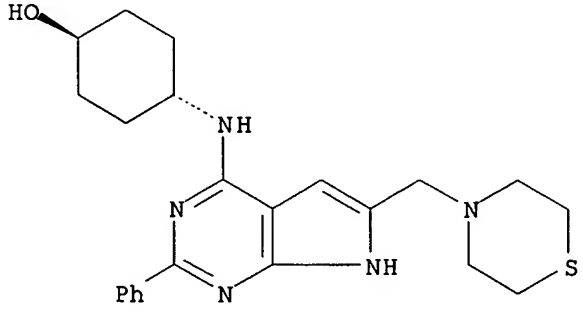
RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 343632-01-9 CAPLUS
CN Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

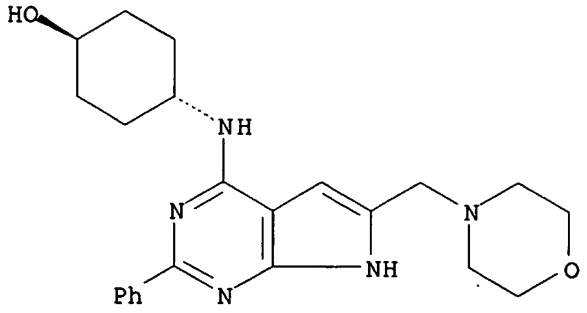
Relative stereochemistry.



RN 343632-02-0 CAPLUS

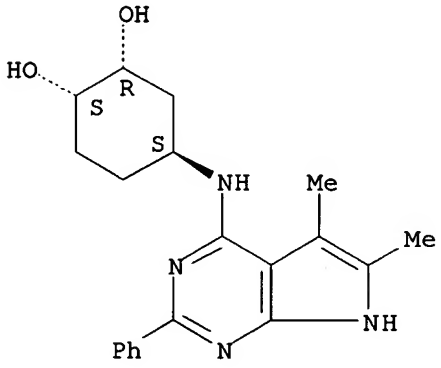
CN Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



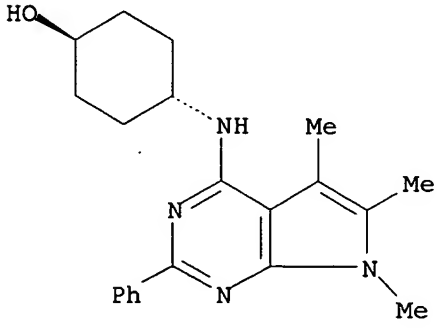
RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



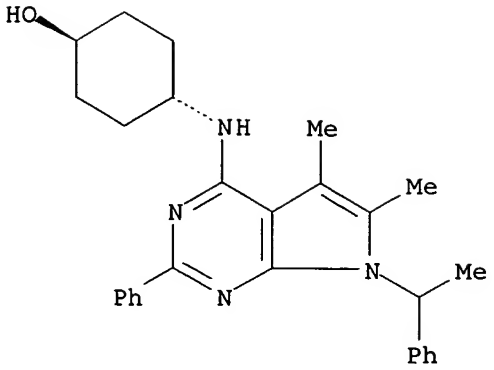
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



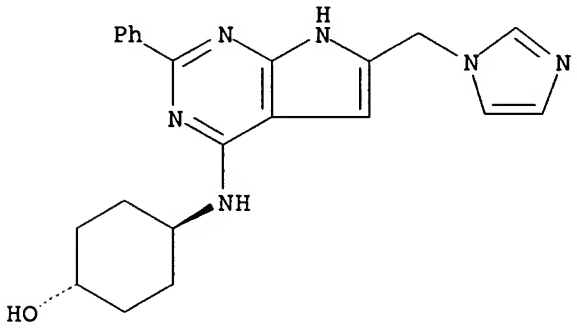
RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



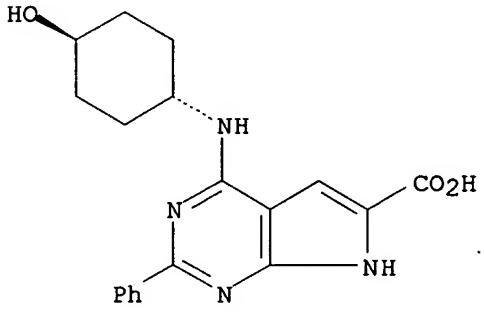
RN 343632-61-1 CAPLUS
CN Cyclohexanol, 4-[[6-(1H-imidazol-1-ylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



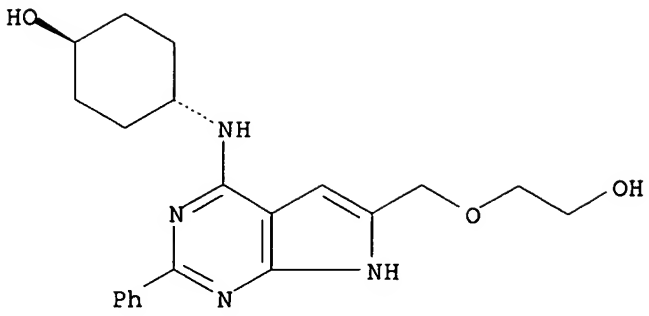
RN 343632-62-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



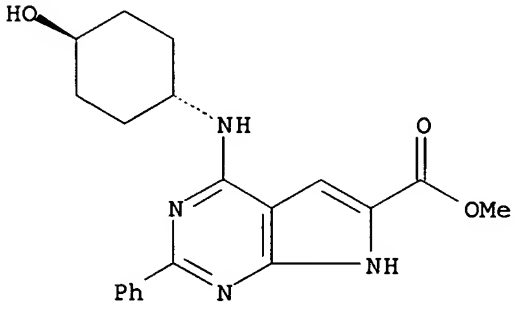
RN 343632-63-3 CAPLUS
CN Cyclohexanol, 4-[[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



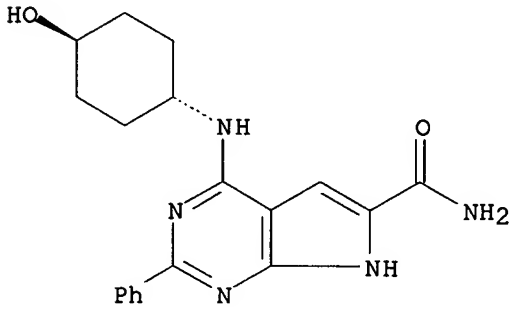
RN 343632-64-4 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



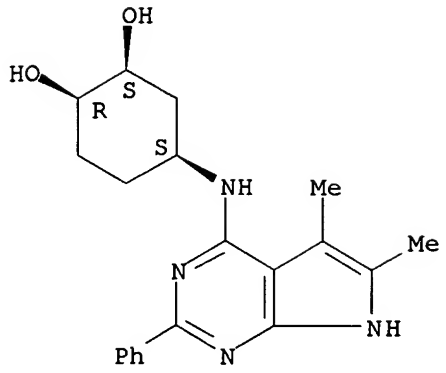
RN 343632-67-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxamide, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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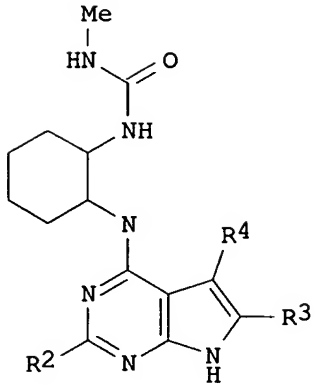

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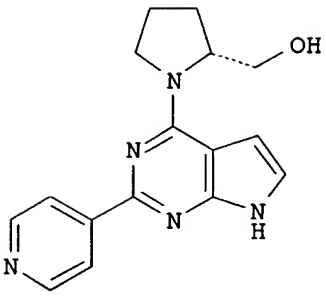


II

AB Title compds. I and analogs [R2 = 5-6 membered aromatic ring; R3-4 = H, alkyl] were prepared Over 100 examples were provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120° for 18 h to yield II in 13% yield after purification Compound I [R2 = Ph; R3-4 = Me] exhibited 10-fold selectivity for binding to the adenosine A1 receptor than to A2a, A2b or A3 receptors. ClogP values were determined for selected example compds. I are useful for the treatment of COPD, allergic rhinitis, etc.

L5 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:416773 CAPLUS
DOCUMENT NUMBER: 135:46190
TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 368 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

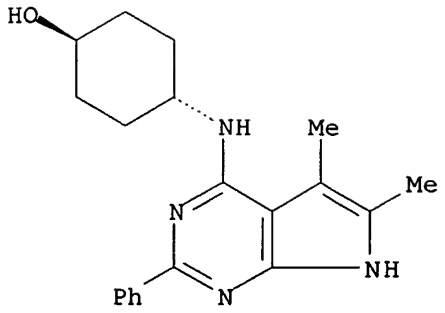
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001039777	A1	20010607	WO 2000-US32702	20001201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6686366	B1	20040203	US 1999-454075	19991202
US 6878716	B1	20050412	US 1999-454074	19991202
CA 2393179	AA	20010607	CA 2000-2393179	20001201
EP 1246623	A1	20021009	EP 2000-988011	20001201
EP 1246623	B1	20060809		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519102	T2	20030617	JP 2001-541509	20001201
AU 784878	B2	20060713	AU 2001-24270	20001201

PRIORITY APPLN. INFO.:	US 1999-454074	A	19991202
	US 1999-454075	A	19991202
	US 1999-454254	A	19991202
	US 1998-87702P	P	19980602
	US 1999-123216P	P	19990308
	US 1999-126527P	P	19990326
	WO 1999-US12135	A2	19990601
	WO 2000-US32702	W	20001201

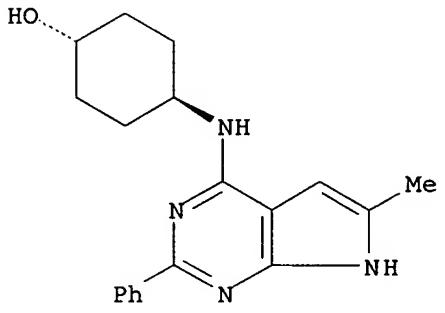
OTHER SOURCE(S): MARPAT 135:46190
IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251945-99-0P 251946-00-6P
251946-01-7P 251946-03-9P 251946-04-0P
251946-05-1P 251946-20-0P 251946-57-3P
251946-58-4P 343632-01-9P 343632-02-0P
343632-03-1P 343632-05-3P 343632-07-5P
343632-61-1P 343632-62-2P 343632-63-3P
343632-64-4P 343632-67-7P 343969-79-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)
RN 246855-41-4 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



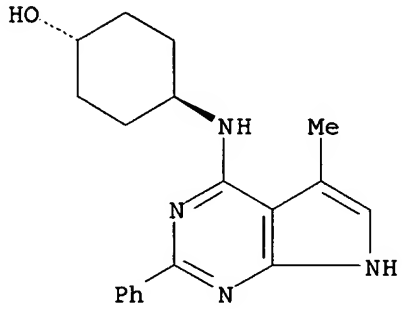
RN 251945-90-1 CAPLUS
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



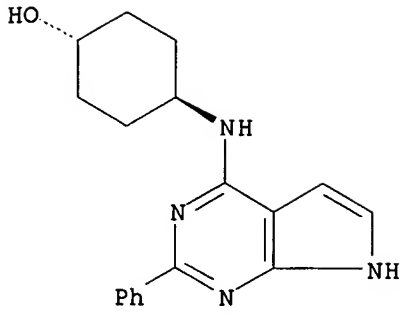
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



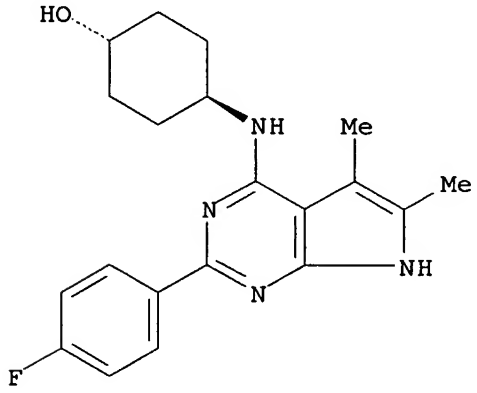
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



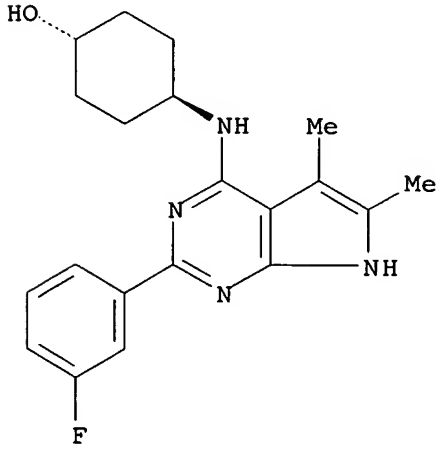
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



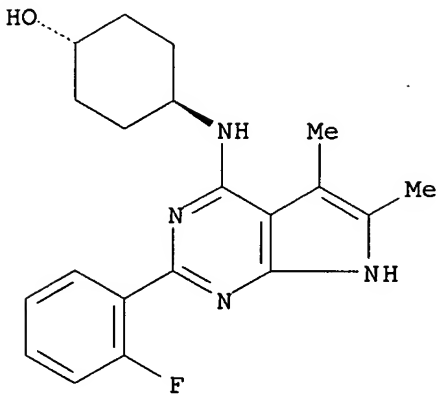
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



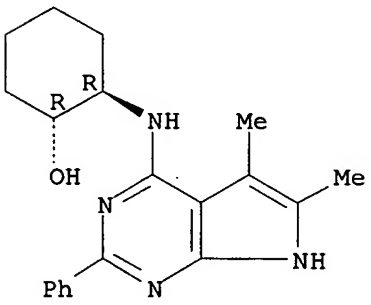
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



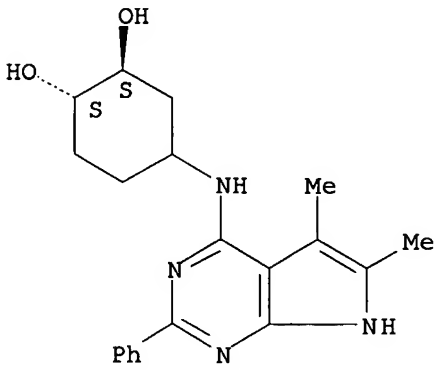
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



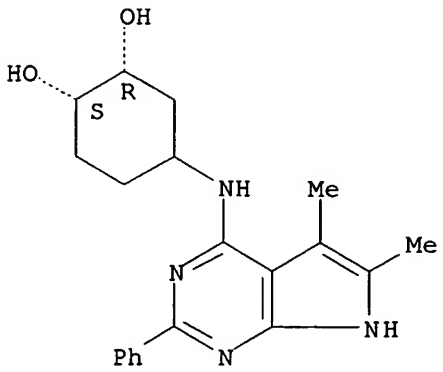
RN 251946-04-0 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



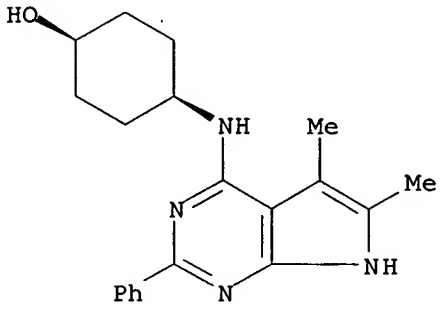
RN 251946-05-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



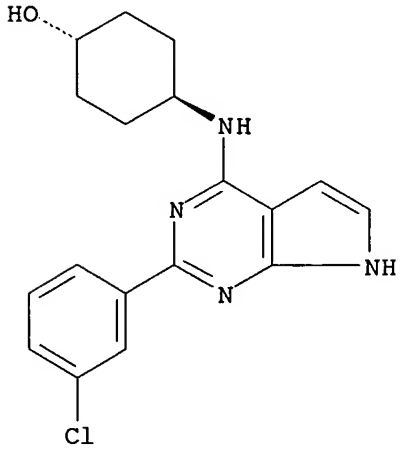
RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



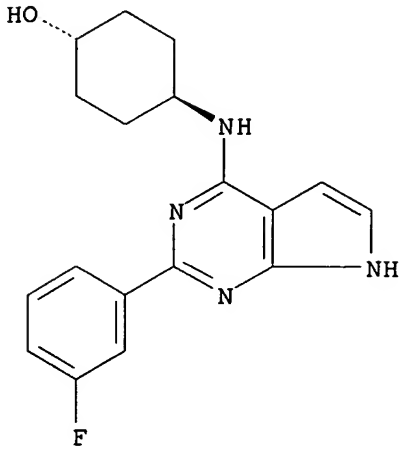
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



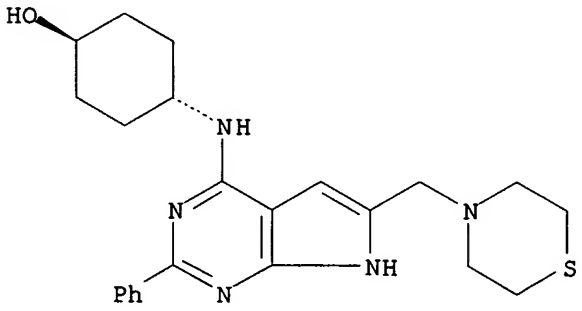
RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



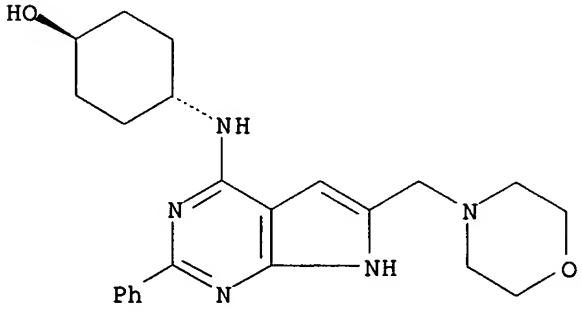
RN 343632-01-9 CAPLUS
CN Cyclohexanol, 4-[[2-phenyl-6-(4-thiomorpholinylmethyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



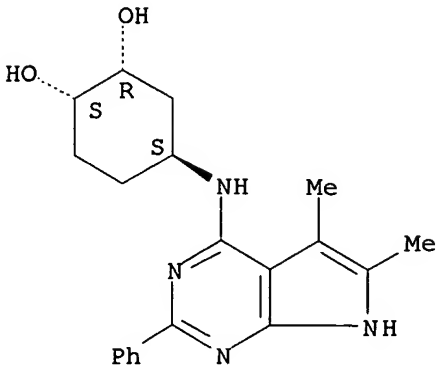
RN 343632-02-0 CAPLUS
CN Cyclohexanol, 4-[[6-(4-morpholinylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



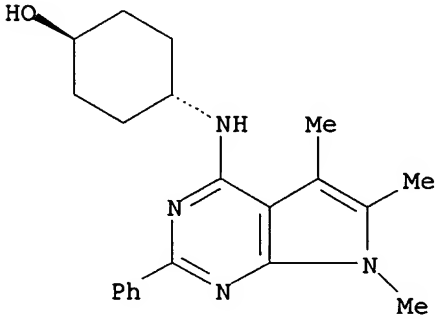
RN 343632-03-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



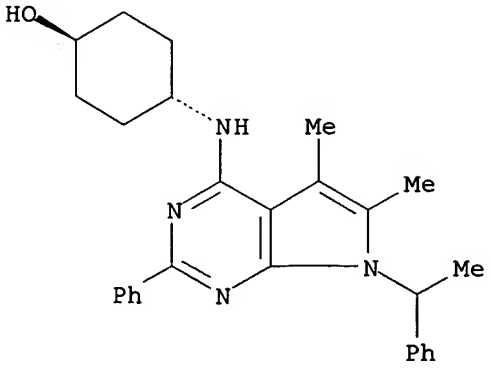
RN 343632-05-3 CAPLUS
CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



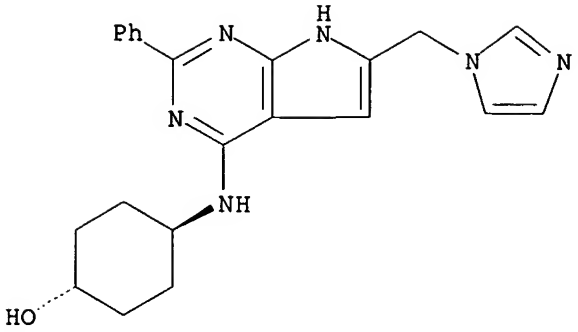
RN 343632-07-5 CAPLUS
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



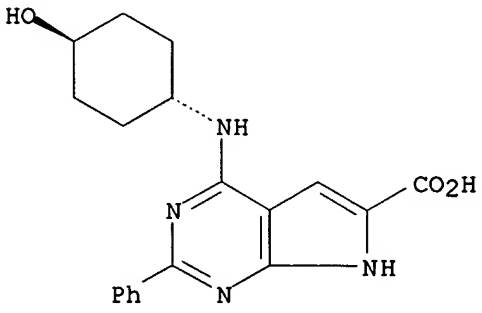
RN 343632-61-1 CAPLUS
CN Cyclohexanol, 4-[[6-(1H-imidazol-1-ylmethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



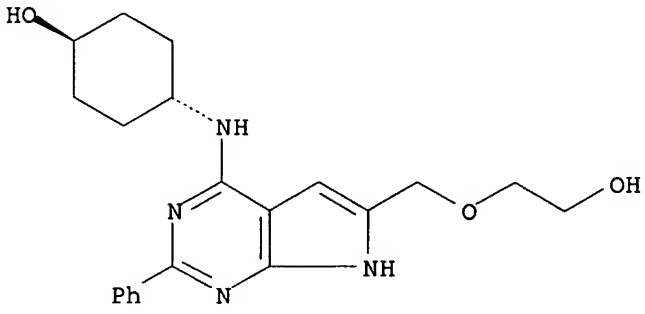
RN 343632-62-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



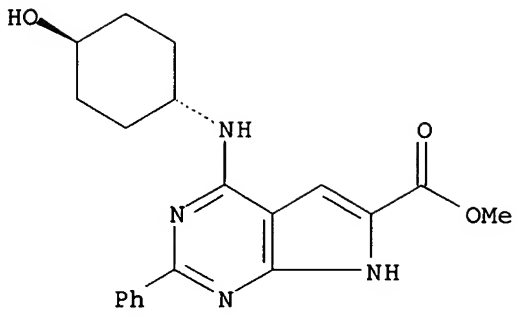
RN 343632-63-3 CAPLUS
CN Cyclohexanol, 4-[[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



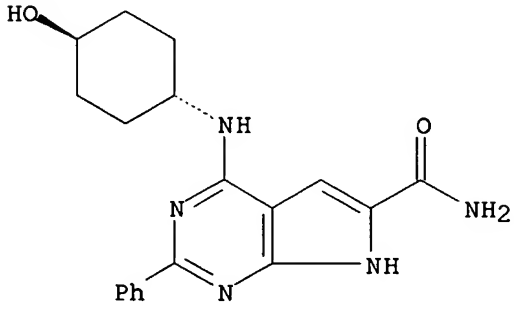
RN 343632-64-4 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



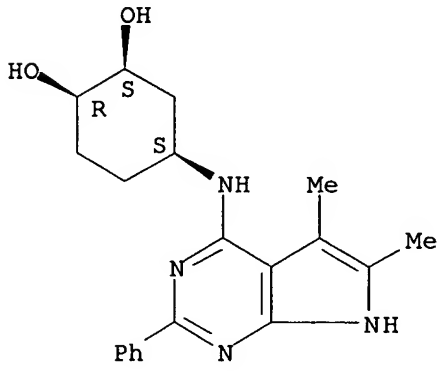
RN 343632-67-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxamide, 4-[(trans-4-hydroxycyclohexyl)amino]-2-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 343969-79-9 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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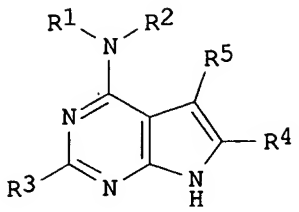

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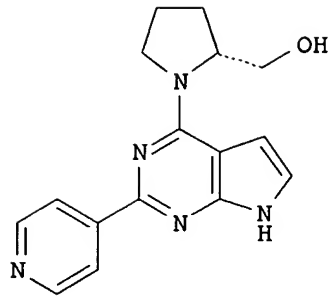


III

AB The synthesis of compds. I, their binding to adenosine receptors and use are described [wherein; R1, R2 = H, (un)substituted alkyl or NR1R2 = (un)substituted 4-8 membered ring; R3 = (un)substituted 4-6 membered (aromatic) ring; R4, R5 = H, (un)substituted alkyl, aryl (with some exceptions)]. Over 100 examples are provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield III in 13% yield after purification Compound I [R1 = AcNHCH2CH2; R2 = H; R3 = Ph; R4, R5 = Me; II] exhibited selective binding to adenosine receptor A1 with IC50 = 82.8 nM. Compound II also had Ki = 9.8 nM (vs. Ki = 7.1 for control ligand 8-cyclopentyl-1,3-dipropylxanthine (DPCPX)). Pyrimidine III binds 5 times more selectively to adenosine receptor A2a than A1, A2b or A3 (no data). Compound I [R1 = AcNH(CH2)4; R2 = H; R3 = Ph; R4, R5 = Me] is 10 times more selective for A3 than the other receptor subtypes. ClogP (calculated partition coefficient between octanol and H2O) values were determined for selected example compds. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease associated with A1, A2a, and A3 adenosine receptors in a subject.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:783937 CAPLUS
DOCUMENT NUMBER: 132:22973
TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): Cadus Pharmaceutical Corp., USA
SOURCE: PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9962518	A1	19991209	WO 1999-US12135	19990601

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,

CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2334200	AA	19991209	CA 1999-2334200	19990601
AU 9942265	A1	19991220	AU 1999-42265	19990601
AU 763658	B2	20030731		
BR 9911612	A	20010206	BR 1999-11612	19990601
EP 1082120	A1	20010314	EP 1999-926107	19990601
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200003513	T2	20010621	TR 2000-200003513	19990601
JP 2002516861	T2	20020611	JP 2000-551774	19990601
NZ 508314	A	20040326	NZ 1999-508314	19990601
US 6686366	B1	20040203	US 1999-454075	19991202
US 6878716	B1	20050412	US 1999-454074	19991202
NO 2000006090	A	20010131	NO 2000-6090	20001130
US 2002028782	A1	20020307	US 2000-728229	20001201
US 6800633	B2	20041005		
US 2005043332	A1	20050224	US 2004-816329	20040331

PRIORITY APPLN. INFO.:	US 1998-87702P	P	19980602
	US 1999-123216P	P	19990308
	US 1999-126527P	P	19990326
	WO 1999-US12135	W	19990601
	US 2000-728229	A3	20001201

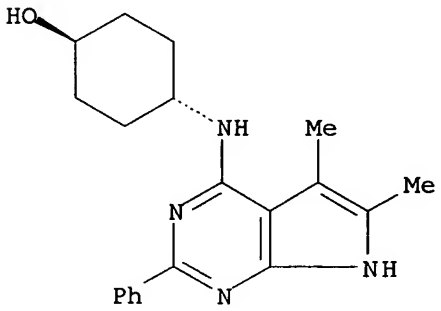
OTHER SOURCE(S): MARPAT 132:22973

IT 246855-41-4P 251945-90-1P 251945-91-2P
251945-92-3P 251945-99-0P 251946-00-6P
251946-01-7P 251946-03-9P 251946-04-0P
251946-05-1P 251946-20-0P 251946-57-3P
251946-58-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)

RN 246855-41-4 CAPLUS

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

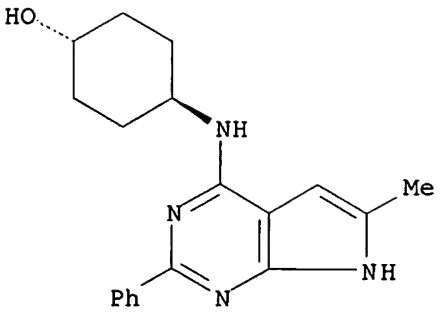
Relative stereochemistry.



RN 251945-90-1 CAPLUS

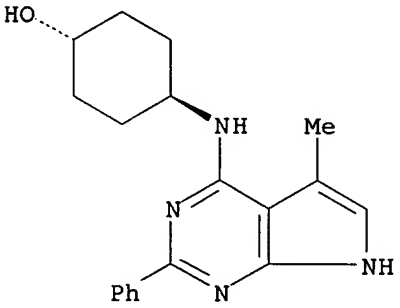
CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



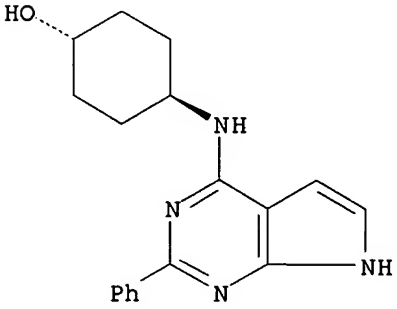
RN 251945-91-2 CAPLUS
CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



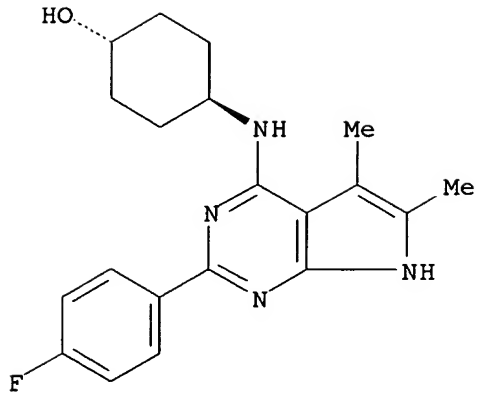
RN 251945-92-3 CAPLUS
CN Cyclohexanol, 4-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



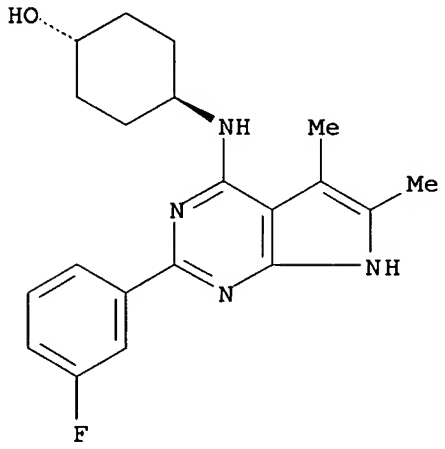
RN 251945-99-0 CAPLUS
CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



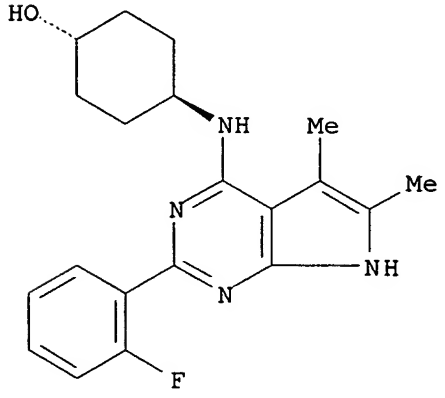
RN 251946-00-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



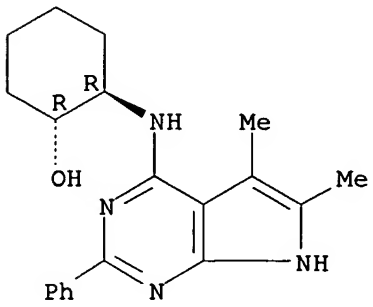
RN 251946-01-7 CAPLUS
CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



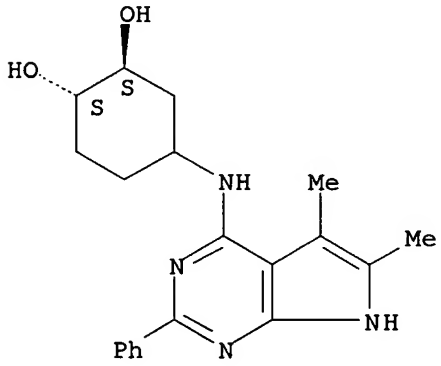
RN 251946-03-9 CAPLUS
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



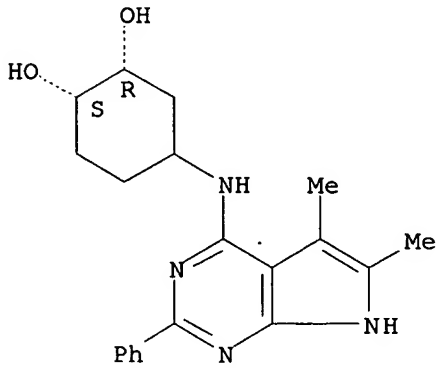
RN 251946-04-0 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-05-1 CAPLUS
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

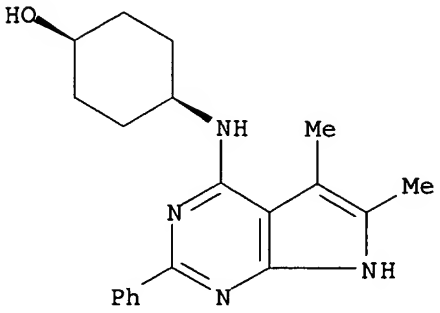
Relative stereochemistry.



RN 251946-20-0 CAPLUS
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-

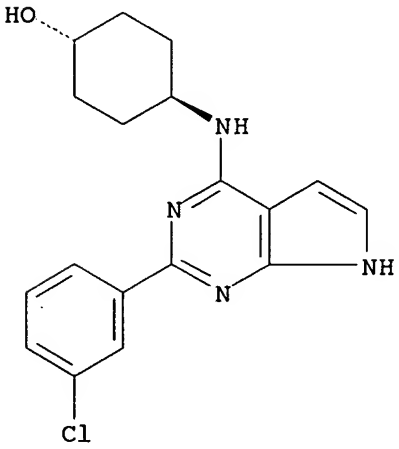
yl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



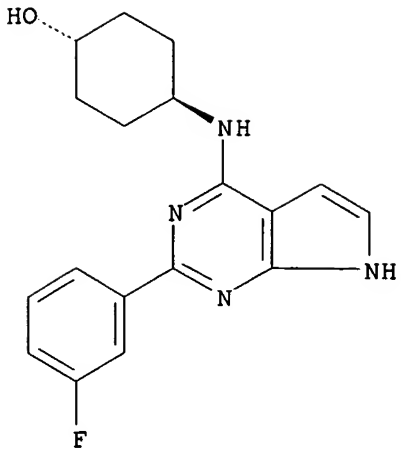
RN 251946-57-3 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 251946-58-4 CAPLUS
CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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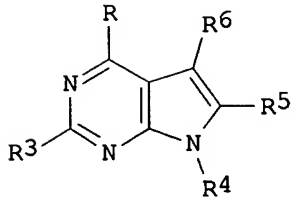


I

AB Title compds. [I; R = NR1R2; R1-R4 = H, alkyl, aryl, etc.; NR1R2 = heterocyclyl; R5,R6 = H, halo, alkyl, aryl, etc.; R4R5,R5R6 = atoms to complete a ring] were prepared Thus, 2- amino-3-cyano-4,5-dimethyl-1-(1-phenylethyl)pyrrole was N-benzoylated and the product cyclized to give, after deprotection and chlorination, I (R3 = Ph, R4 = H, R5 = R6 = Me)(II; R = Cl) which was aminated by trans-4-hydroxycyclohexylamine to give II (R = trans-4-hydroxycyclohexylamino). Data for biol. activity of I were given.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:571295 CAPLUS

DOCUMENT NUMBER: 131:281026

TITLE: Selective A1-adenosine receptor antagonists identified using yeast Saccharomyces cerevisiae functional assays

AUTHOR(S): Campbell, Robert M.; Cartwright, Craig; Chen, Wei; Chen, Yong; Duzic, Emir; Fu, Jian-Min; Loveland, Michelle; Manning, Ron; McKibben, Bryan; Pleiman, Christopher M.; Silverman, Lauren; Trueheart, Joshua; Webb, David R.; Wilkinson, Vicki; Witter, David J.; Xie, Xiaobing; Castelhano, Arlindo L.

CORPORATE SOURCE: Cadus Pharmaceutical Corporation, Tarrytown, NY, 10591, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(16), 2413-2418
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

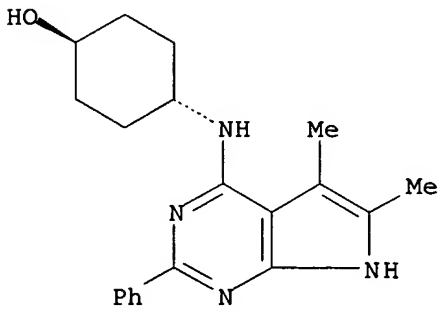
LANGUAGE: English

IT 246855-41-4P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(selective A1-adenosine receptor antagonists identified using yeast functional assays)

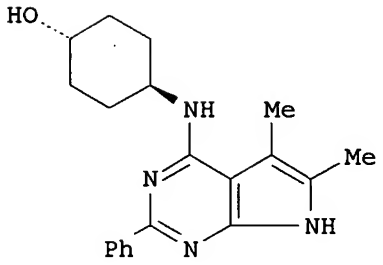
RN 246855-41-4 CAPLUS

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



I

AB Evaluation of a biased "library" of pyrrolo[2,3-d]pyrimidines using yeast-based functional assays expressing human A1- and A2a-adenosine receptors, led to the A1 selective antagonist I. A direct correlation between yeast functional activity and binding data was established. Practical compds. with polar residues at C-4 of the pyrrolopyrimidine system required H-bond donor functionality for high potency.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	66.89	238.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-9.75	-9.75

STN INTERNATIONAL LOGOFF AT 06:38:10 ON 23 SEP 2006